

PROCEEDINGS OF THE WORKSHOP
ON THE
PRESENT STATUS
AND
FUTURE DEVELOPMENTS
OF SOLID STATE
CHEMISTRY AND MATERIALS

January 15 - 16, 1998

Arlington, Virginia

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Introduction to the Report

There is currently much discussion concerning the appropriate National paradigm for support of research. Accordingly, it seems especially important to evaluate recent advances and to articulate future challenges and opportunities in particular research areas. This is especially true of the rapidly emerging and changing field of Solid State Chemistry and Materials which has undergone explosive growth, both in industrial and in academic laboratories, over the last decade. Part of this trend may be attributed to the discovery of new materials with important technological applications, and part of this is a reflection of the growth in intellectual scope of the field whose boundaries have expanded considerably: materials chemistry has emerged as a discipline in its own right, closely intertwined with activities traditionally recognized being in the domain of solid state chemistry. It therefore appeared timely to institute a workshop on the Present Status and Future Developments of Solid State Chemistry and Materials to survey the many different activities in this field and to outline emerging and exciting trends, needs, and challenges.

The following guiding principles were adopted for the development of an agenda appropriate to a Workshop; these were developed at NSF as detailed in Appendix A:

- Define research opportunities in the field of solid state chemistry and materials.
- Identify the most important multidisciplinary areas for involvement by the solid state chemistry and materials community.

- Determine novel roles for the Solid State Chemistry and Materials community that will advance educational and training opportunities for future scientists, engineers, and technicians.
- Develop new approaches that allow for the more effective and efficient conduct of research and educational activities.

The Workshop was held January 15-16, 1998 at the NSF headquarters in Arlington, VA. Thirty-four individuals participated in various presentations; twenty-four registered individuals were in attendance as observers, and approximately thirty-five additional individuals, mostly NSF personnel, were present at various times during the Workshop. A very important component of the Workshop was the preparation of the Conference Proceedings as a report that was to receive wide distribution. One of the aims of this document is to encourage continuing wide-ranging discussions of current advances and research opportunities in this area which is of great importance to our national welfare.

The Workshop began on Thursday, January 15, 1998, with four topical presentations in the areas of: *Strategies for New Materials Discoveries*, R. Cava, Coordinator; *Structure Properties Relations*, S. Lee, Coordinator; *Hybrid Materials and Interfaces*, M. D. Ward, Coordinator; *Societal Needs and Technological Opportunities*, D. W. Murphy, Coordinator; other invited participants in the topical presentations are listed with the Topical Area Reports beginning on page 14. Small follow-up group discussions on these topics were scheduled for the afternoon; at the same time, the Panel Discussion Groups met to plan their presentations for the next day. In the evening, a meeting was held at which the various topical coordinators presented their preliminary outlines for the report. Observers were encouraged to participate in all the discussion meetings and to ask questions during the presentations.

On Friday morning, January 16, the following panel discussions were held: *Education and Training*, S. M. Kauzlarich, Coordinator; *Facilities and Resources*, T. M. Swager,

Coordinator; "What is Materials Chemistry?", S. I. Stupp, Coordinator; other invited participants in the panel discussion presentations are listed with the Panel Discussion Reports beginning on page 52. In the afternoon, the participants in the topical presentations and panel discussions met to work out a preliminary version of the reports in their respective areas.

The various coordinators then met with T. E. Mallouk and J. M. Honig on Saturday morning, January 17, to complete their work on a draft version of their report.

It should be emphasized that all areas that comprise Solid State Chemistry and Materials activities could not be covered in the limited time frame of the Workshop. These topics fell largely in the rubrics of *chimie douce*, organometallic chemistry, polymer chemistry, and some aspects of nanoscale and mesoscale research. Many of these topics were taken up in an earlier Workshop on Interdisciplinary Macromolecular Science and Engineering, organized by S. I. Stupp and held May 14 - 15, 1997, and in a Workshop on Materials Design and Processing at the Nano- and Mesoscales through Self-Assembly, organized by M. Tirrell, and held on January 13 - 14, 1998. Further workshops in the Solid State Chemistry and Materials area are planned in subsequent years, with a complete rotation of personnel, so as to minimize any built-in prejudices that could hamper the development of the field. In view of the above, it is particularly important to take the recommendations in the present report as an indication of possible future research opportunities and additional funding initiatives. Not all worthwhile activities could be considered in the limited Workshop agenda. Thus, if ongoing research in the Solid State Chemistry and Materials area is not specifically mentioned in the present report, this is not to be construed as indicating that such activities should be de-emphasized or discontinued. This report is meant to stimulate continuing community discussion and planning; the Workshop format is perhaps only one of several options under which such vital discussions can occur.

EXECUTIVE SUMMARIES

STRUCTURE-PROPERTY RELATIONSHIPS - S. LEE

Computer-based calculational projects form an important tool for the adjustment of variables that optimize characteristics linking the synthesis of all types of materials with desired physical properties. Tools available for this purpose and goals for successful implementation include:

- User-friendly data bases (enumerated in the text) which survey compounds, reactions, physical properties, and structures, complete with codes that allow processing and statistical studies.
- The construction of quantum structure maps, based on atomic parameters, as a function of composition; these are useful for the prediction of the existence of new phases and of their properties.
- Theory and computation. Just as experimental data are currently used to model many physical properties, so theoretical calculations are expected to influence the generation of new materials and their properties.
- The development of interconnective information encompassing virtually all steps in materials development. More collaboration between theorists and experimentalists is expected to strengthen this very important process.

Density functional theory is a very important tool in the achievement of the above-mentioned goals. Of great value would be improvements in the empirical and semiempirical methodologies appropriate to the analysis of very large collections of atoms that begin to simulate the solid state. A listing of factors involved is found in Table 1, page 17. Problems considered heretofore as inaccessible have now become tractable; a listing is provided in the text.

Recommendations for the future include emphasizing the value of strong collaboration between theoreticians and

experimentalists to resolve specific materials issues. Experimentalists should be assisted in learning how to do their own calculations rather than relying exclusively on theoreticians. Towards this goal it is necessary to develop more user-friendly codes, organizing tutorial workshops, and making supercomputing facilities more readily available to nonspecialists.

DISCOVERY OF NEW MATERIALS - R. CAVA

Many different innovative methods are presently in use to discover new materials by exploration of uncharted regions of thermodynamic stability or by materials processing in regions of metastability. Robot-assisted combinatorial synthesis is also being more commonly employed. Methods of choice for synthesis include templating, use of extreme operating conditions, low temperature flux and hydrothermal techniques, self assembly, combinatorial chemistry, soft chemistry, and electrochemistry. The creative use of such techniques is well illustrated by the world-wide research and development efforts in the area of high temperature superconductors.

Two strategies in use for discoveries are:

- The chemistry-driven approach, which concentrates on reactions, compounds, or structural motifs, with lesser emphasis on properties.
- The properties-driven approach, with emphasis on basic science or technological applications of materials, with the goal of optimizing their properties.

Both types of effort are required to advance solid state chemistry and materials research.

New materials, such as the high temperature superconductors, lead the way in technological progress, revealing new phenomena and/or forcing a reevaluation of what

was thought to be understood. A listing of such materials discovered in the last 25 years is supplied in Table 2, page 24; the obvious high degree of interest and activity in this area continues unabated. It is therefore important to encourage further active research leading to the discovery of new materials. A vast area is still unexplored; for example, only 0.01% of all possible quaternary intermetallic compounds have so far been investigated. Maintenance of core expertise in such an endeavor is absolutely essential, with particular emphasis in following up new leads as these arise.

As also emphasized elsewhere, a high degree of interdisciplinary effort should be encouraged to attain the above goals, centered on the training of students in areas outside the normal chemistry curriculum. NSF should be encouraged to expand focused research programs involving solid state chemistry interacting with contiguous disciplines. The successful establishment of such programs in academia should be recognized as an important consideration in tenure decisions at universities.

More effort should be placed on the synthesis of new materials by design, rather than on finding out what materials can be made. This requires more studies on reaction mechanisms, as well as computer-aided methodologies which can predict properties from first principles. As also stated elsewhere, user-friendly computer programs will greatly assist in this task.

HYBRID MATERIALS - M. D. WARD

Hybrid materials play an increasingly dominant role in the synthesis of future products generated through Solid State Chemistry and Materials research and development. A major problem in this development is the proper control of interfaces separating dissimilar components. Thus, future Solid State

Chemistry and Materials research must adequately deal with new interface design principles and with the development of functional molecular entities capable of controlling interfacial properties. This also requires structure and property design at small length scales so as to achieve complex hierarchical structures at large length scales. Examples of emerging activities include thin film structures, layered compounds, as well as three dimensional crystalline and disordered networks. Synthetic methods generally involve the 'bottom up' approach by (a) deposition of films, (b) use of molecular building blocks for synthesis of self-assembled monolayers, (c) sol-gel synthesis, (d) organic structure or surfactant-directing agents, (e) use of colloid chemistry and intercalation. In these activities templating provides exquisite control over synthesis of hybrid materials with desired properties. Such operations are generally carried out under conditions far removed from equilibrium at low temperatures to ensure stability.

The above operations require characterization capabilities with a new generation of tools capable of operating in the microdomain, especially microscopic imaging and topography, probing buried interfaces, developing new methods for detection of defects and trace analysis, and developing user-friendly theoretical tools for modeling interfaces. Future challenges include the establishment of structure-property relationships involving several length scales, studies of non-covalent forces governing interfacial structures, learning how to control interfacial stability, developing better computational strategies, and systematic development of new materials.

SOCIETAL NEEDS AND TECHNOLOGICAL OPPORTUNITIES -
D. W. MURPHY

Societal needs and technological opportunities may be addressed by understanding, controlling, and predicting properties of solids, so as to produce new materials with superior properties. Solid State Chemistry and Materials activities have impacted on everyday activities in diverse areas such as health, energy, environment, electronics and communications, transportation, security, scientific breakthroughs, and education. We depend both on sudden burst of insight and on logical extension of current technologies to attend to societal needs.

Technologies dependent on a Solid State Chemistry and Materials knowledge base are growing as fast as 50% per year, which requires a stream of steady Solid State Chemistry and Materials research activities that largely evolve and grow in response to emerging technological needs. This calls for adventurous research activities, proper allocation of resources, skill sets that allow new knowledge to be acquired, and investigations into new areas. The US ranks high in Solid State Chemistry and Materials portfolios, but is seen lagging in fundamental research that produces new materials. Another danger signal is the scaling back of fundamental research in the industrial sector. Mechanisms to reverse this trend should be encouraged, and serious attempts should be made to remove obstacles such as limiting intellectual property rights. Steps such as providing sabbatical leaves of absence, encouraging scientific exchanges, and instituting more tutorials are also important in redressing the problem.

A detailed listing of representative accomplishments and opportunities in the Solid State Chemistry and Materials area is furnished in Table 4, page 51, in the body of the report.

PANEL ON EDUCATION - S. M. KAUZLARICH

Many undergraduate students go through their curriculum without ever being introduced to the chemistry of extended structures. As a remedy it is important to:

- include Solid State Chemistry and Materials subject matter in elementary courses,
- train teachers to appreciate and foster the subject area,
- foster interchange of resources and research capabilities among researchers in the field,
- publicize by outreach highlights in the Solid State Chemistry and Materials area.

Listed in the body of the report are a number of NSF-sponsored educational projects which the Panel identified as having been highly successful at the K-6 grade level, the middle and high school range, and for the college curriculum; most relevant and notable among these is the Summer Research Program in Solid State Chemistry for Undergraduate Students and College Faculty, which has been highly successful. Materials intensive courses are identified in the main body of the report, as well as instructional materials, appropriate resource articles, models, and the like. The Panel also provided information on (a) instructive articles in the related areas of polymer and materials science, (b) listings of research efforts in these areas, (c) descriptions of research opportunities in these fields, (d) the present status of the initiation of the IGERT program at NSF.

The Panel further issued several recommendations:

- Guidance should be provided to prospective students in the Solid State Chemistry and Materials area through workshops, textbooks, American Chemical Society-certified courses, team-taught instruction, and Ph.D. programs specific to the area.
- Special curricula should be set up emphasizing undergraduate research programs that are supervised

by small collaborative teams of faculty in different departments or even different campuses.

- Current NSF-sponsored research should include an educational component.
- The Solid State Chemistry and Materials activities should have wide representation at national meetings of professional societies through plenary lectures and tutorials involving cutting-edge work in the field.
- A web site should be instituted on teaching resources, as should faculty web sites, research and co-op opportunities and fellowships, and research interactions between faculty and personnel in national laboratories.
- An effort should be made to provide the public with better information of activities in the Solid State Chemistry and Materials area through articles, other means of information dissemination, and involvement in local school science projects.

PANEL ON FACILITIES AND RESOURCES - T. M. SWAGER

In its meeting the Panel dealing with Facilities and Resources commended NSF for effectively promoting science and innovation with limited resources. The overall consensus is that the Division of Materials Research maintains a multifaceted portfolio that is responsive to scientific needs and opportunities. Changing times have required new mechanisms for supporting young faculty (CAREER), support for interdisciplinary research teams (STC and MRSEC), funding exploratory research (SGER), and increased equipment resources. The balance of these programs is considered to be carefully managed so as to produce the maximum impact from NSF dollars. The Workshop participants felt that the average grant size should not be increased if this leads to a reduction in the number of individual grants, for which the success rate is already dangerously low. This community also favored a mail review system in which reviewers are asked to handle proposals in

batches, so as to provide a basis for comparison of the relative merits of different proposals in the same area. While no specific redistribution of funds in DMR were recommended, the Workshop participants and the members of the facilities and resources panel voiced strong support for some particular initiatives. DMR's recent success in effectively doubling the IMR budget was warmly appreciated, and is a proper response to the ever expanding role of sophisticated equipment and facilities in the execution of materials research.

The Workshop participants further felt that there was a reasonable balance in the allocation of funds to large research centers and individual researchers. However, information concerning access by outsiders to work station at various centers should be made more readily available to the community at large than is presently the case. The Workshop panel and the participants examined presently available large scale sophisticated equipment and identified further opportunities for equipment initiatives, including complex synthesis equipment (furnaces, molecular beam epitaxy, etc.), facilities for combinatorial materials synthesis and screening, high field (900MHz) NMR, and equipment for the characterization of materials under extreme conditions (high/low temperature, high pressures).

The possibility of creating remote access capabilities that directly tie into research centers should be carefully examined and then implemented. A new initiative should be pursued which allows individual scientists to purchase modern equipment too costly to be included in standard grant proposals, and yet not large enough to qualify for the current equipment grant proposal. This is deemed to be important because of increasing needs for sophisticated equipment of this type in the laboratory of individual researchers.

The Workshop community also supported the establishment of a postdoctoral fellowship program in DMR, which would assist in

the training of future researchers. The panel felt that an expansion of cooperative inter-agency agreements would represent an important opportunity for graduate fellowship support. Mechanisms for the more effective utilization of DOE and NIST facilities in NSF sponsored research should also be investigated.

**PANEL ON DEFINING WHAT IS MATERIALS CHEMISTRY. -
S. I. STUPP**

A panel was organized to pose and address the question "What is the intellectual scope of materials chemistry?" through interactive discussion. It was also of interest to this panel to establish the relations between materials chemist and other well established disciplines, such as chemistry, materials science, chemical engineering, and solid state chemistry. Materials Chemistry is generally taken to be a discipline concerned with the understanding and control of functional condensed matter from a chemical perspective.

Materials utilized by society need to be processed into macroscopic functional forms; their chemical nature and complexity will evolve over time. Therefore practitioners of materials chemistry must have growing interactions with all disciplines of chemistry and with other fields of science and engineering. These interfacial, interdisciplinary efforts are currently experiencing rapid growth. There is also general agreement in the community that materials chemistry is an exciting area of scientific opportunity that will profoundly affect our increasingly technological society. Its importance is clearly demonstrated by such trends as the increasing number of journals and publications in materials chemistry, by the increasing number of faculty who are involved in materials research, by the growing interest of funding agencies in the welfare of the field, and by the materials chemistry materials

produced by the top 100 chemical companies in the US. The top six of these companies have presently a significant stake and interests in materials; the number of companies among the 100 whose products are mainly related to materials chemistry can be estimated conservatively to be as high as one third. In terms of chemical sales the majority of these companies rank among the top fifty. In light of the above, academics can play a very useful and supportive role in the industrial development of materials chemistry and NSF should provide adequate support of research and foster industry-academic cooperation in this area.

TOPICAL AREA REPORTS

I. Structure-Property Relationships - S. Lee; Coordinator, M. Greenblatt, T. Hughbanks, A. Rappe.

One may expect that computation will play an even more essential role in the solid state community than it now plays among molecular chemists, because of the fundamental importance of properties and structure-property relations plays in the further development of solid state chemistry.

Structure-property relationships constitute one of the core components of the solid state chemistry mission, linking the synthesis of new inorganic, organic, and mesoporous systems with the desired functional electronic, optical, magnetic and chemical properties of actual materials. Therefore, structure-property relationships are an integral part of most and perhaps all solid state chemistry and materials chemists' research programs. Detailed structure-property studies have led to the optimization of high T_c superconductors, fast ion conductors, dilute magnetic semiconductors, materials undergoing metal-insulator transitions, microwave ferrites, and the like.

While the core component of structure-property relationships continues to be the careful manipulation of variables, such as composition and structure in the optimization of properties, one can identify three key efforts that will generally facilitate such work:

- The emergence of computerized data bases
- Quantum structure maps
- Quantum based and empirical energy calculations.

These three key efforts can be implemented in the following four emerging technologies and techniques:

1. The utility of user-friendly and cost effective databases cannot be understated. Paradigms for user-friendly system include the Cambridge Structure Database and Beilstein. These databases allow access to every phase of organic chemistry, from a catalog of all reported reactions and compounds, to physical properties and detailed solid state structures. Equally important databases for the inorganic and physical community include Landoldt-Börnstein, Gmelin, ASM phase diagrams, ICSD and the Pearson crystallographic data. It is not just the availability of the data that is important, but also the development of codes which allow for processing and statistical or comparative studies.

2. A second significant new method for the study of structure-property relations has been the introduction of quantum structure maps. In this approach one uses a set of atomic parameters, based on concepts such as orbital size, ionization potentials, or more phenomenological variables. These then are used to create maps as a function of composition for the physical properties of interest. A partial list of properties studied include phase stability, structure type, and superconductivity. In the category of structure type, for example, structure maps have been used for the successful prediction of new quasicrystalline phases.

3. The third emerging area in structure-property studies, theory and computation, can potentially revolutionize the field of structure-property relations. This is described below in more detail.

4. A further evolution appears to be emerging in the range of structure/property relationships which increasingly involve interconnections between all steps of the materials development process, from the very first, generally synthesis, to the very last, the production of processed and shaped material goods. There is therefore a growing awareness on the part of solid state chemists concerning the physical, engineering, and

economic properties of the materials they study. Collaborative interdisciplinary work further strengthens this process.

Theory: Its role in synthesis, structure and properties.

There has been a recent revolution in solid state theory with the advent of computationally accessible quantum methods. Currently accessible systems include those with 10^2 atoms/unit cell. This is an order of magnitude greater than the size of systems accessible to calculations a decade ago. A similar advance in computational power is anticipated in the decade ahead.

The current status of quantum methods in solid state systems resembles that prevailing in molecular chemistry a decade ago. Today, theory forms an integral part of molecular chemistry. Experimentalist in molecular chemistry routinely carry out calculations on properties such as heats and energies of reactions, vibrational frequencies, transition states, NMR chemical shifts, and polarizabilities. In the next decade theory could have a similar impact and profile in solid state chemistry. For some properties, and for a wide range of compositions and structures, solid state chemists will view computational chemistry as an invaluable tool. One may expect that computation will play an even more essential role in the solid state community than it now plays among molecular chemists, because of the fundamental importance of properties and structure-property relations in the further development of solid state chemistry - a field which is driven by new materials and new materials properties.

One of the engines driving the transformation of solid state theory has been improvements and systematization in density functional theory. Ab-initio pseudo-potentials, non-local corrections, quantum dynamic methodologies, and improved computational speed, have collectively greatly enhanced the

accuracy and range of density functional theory; this trend will undoubtedly continue in the future. By now a wide variety of physical characteristics have been developed within the context of density functional theory which are listed in the top part of Table 1. Even more exciting are the presently emerging capabilities which are tabulated on the right-hand side of the Table.

Table 1. Density functional theory capabilities

Established Capabilities	Emerging Capabilities
Bond Lengths and angles within 1%	Temperature dependent structural phase transitions
Vibrational frequencies within 10%	Prediction of new moderate sized structures
Volume-pressure phase diagrams	Ferroelectric phase transitions
Ordering of structural alternatives	Binding of guests on surfaces and porous solids
Static dielectric constants	Ion transport in crystalline solids
Band gaps	Scanning tunneling microscopy images
Angle resolved photoelectron spectra	Piezoelectric properties
Electrochemical potentials	Nonlinear optical properties
	Nuclear magnetic resonance chemical shifts

Of perhaps equal importance are improvements in empirical and semi-empirical methodologies, where more precise force fields and efficient N-scaling, together with enhanced computer power, has permitted calculations within tight-binding theory involving 10^4 atoms, and for molecular dynamics, involving as many as 10^6 atoms. A rough schematic illustrating the interplay between type of theory, size of system and relative accuracy is provided in Figure 1.

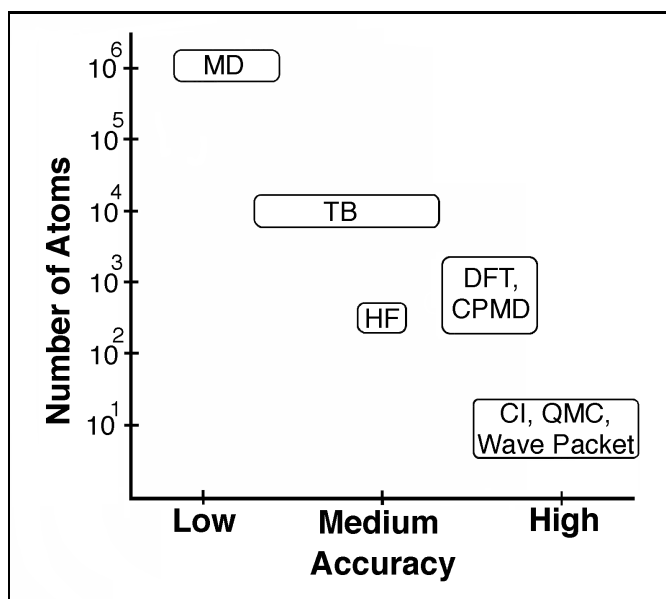


Figure 1. A theoretical hierarchy: size vs. accuracy

The result of these theoretical and computational developments is that problems heretofore inaccessible to calculational treatment are now becoming tractable, allowing theory to provide useful guidance. Molecular dynamics capabilities soon to be available may provide atomic level resolution of interfaces in liquid crystals, block copolymers, and other hybrid materials. With quantum molecular dynamics one could potentially calculate oxygen transport through ceramics. For intermetallic investigations prior to synthesis, density functional theory could differentiate between chemically reasonable alternatives. In pillared clays or intercalation compounds such calculations could provide orientation and binding sites of guest species. First principles techniques could also be used in the design of low band gap conducting polymers.

Both experimentalists and theorists sense the synergism which would come from closer interaction. One may therefore anticipate collaborative work by experimental and theoretical materials chemists aimed at the resolution of specific materials

issues. As the solid state field progresses, much as in molecular chemistry, accurate quantum calculations will be carried out by groups primarily involved in experiment, and not just by theoreticians. The development of user friendly codes, the organizing of tutorial workshops, and the generalized availability of supercomputing facilities is strongly urged to hasten this latter development. Theory should therefore be viewed as an integral and fundamental component of solid state chemistry and materials.

**II. The Discovery of New Materials - R. Cava;
Coordinator, R. Haushalter, M. Kanatzidis.**

The combination of various materials discovery strategies provides the basis for the advancements made in the understanding of the complex relationships between composition, structure and properties that lie at the heart of solid state and materials chemistry.

Where we are:

The discovery, characterization and understanding of new materials is at the heart of solid state and materials chemistry. This activity is pursued vigorously at universities, national laboratories and industrial laboratories, in the U.S. and throughout the world, in both group and individual research programs. The new materials discovered by solid state and materials chemists play an essential role in both fundamental and applications oriented research and development programs in a broad range of scientific disciplines and technological systems. Many advances in understanding the fundamental issues in condensed matter physics, for example, are derived from the physical characterization of new materials. In addition, many of the sophisticated technologies of the future will depend on the

discovery and development of new materials to replace those presently known, which will eventually prove inadequate, or will lead to the implementation of systems previously impossible of realization due to the limitations of the materials now in use. The rapidly growing recognition of solid state and materials chemistry in the past ten years as playing an essential role in many larger multidisciplinary research areas is an indication of its vitality and emerging importance.

When considered in the context of the larger field of chemistry, solid state and materials chemistry as a sub-discipline is experiencing a rebirth. As a consequence, and also due to the complexities which naturally arise from the many-body interactions which occur in extended structures in condensed matter, researchers are presently actively engaged in the process of discovering and developing the relationships between the compositions of materials and their structures. At the same time, their structures and their physical properties are being explored. The growth of the field brings with it the introduction of new synthetic techniques. The development of techniques for the control of structure on length scales between those of atomic scale structures (tens of angstroms) and microstructures (microns) has greatly broadened the range of materials studied by solid state and materials chemists and stimulated forefront multidisciplinary research.

A wide variety of synthetic methods are presently being pursued in innovative ways to discover new materials. These generally either lead to new regions of thermodynamic stability previously not available for synthesis, such as high temperatures and pressures, or access to kinetically stable phases synthesized at significantly lower temperatures and milder conditions. Chemists are increasingly able to exercise more control over structural outcomes. The very recent introduction of robot-assisted combinatorial synthesis to the field has opened larger possibilities for the discovery of

materials with specific physical properties. Some of these methods include:

- *molecular templating*, which allows the preparation of microporous and nanostructured materials,
- *synthesis under extreme conditions of temperature and pressure* which yield new thermodynamic compositions and structures,
- *low temperature flux and hydrothermal methods*, which defeat kinetic limitations of low temperature to access new otherwise unstable phases,
- *self assembly*, which allows the formation of hierarchical structures of hybrid materials,
- *combinatorial chemistry*, which allows the parallel synthesis and screening of many materials in the pursuit of optimal physical properties,
- *high gas pressure reactions*, which allow the synthesis of phases with unusually high chemical activities of ordinarily gaseous components,
- *soft chemistry - chimie douce*, which allows the synthesis of metastable phases,

and

- *electrochemistry*, which allows the formation of oxidized or reduced phases otherwise inaccessible.

The creative implementation of these synthetic techniques has often had a wide ranging effect on fields outside solid state chemistry. The use of the high pressure synthetic method in research on copper oxides is a good example of the dramatic effect that a newly applied method can have on a field (Figure 2). After the initial peak in the number of discovered superconducting compounds in 1988, when a large number of groups throughout the world were actively looking for new high T_c materials, there is a secondary peak in 1993, extending for several additional years. The large number of new materials resulted from the realization that new phases would become thermodynamically stable under high temperature, high pressure conditions. This example shows the great potential for solid

state and materials chemistry to influence the course of discovery in an important international research area outside its own direct boundaries.

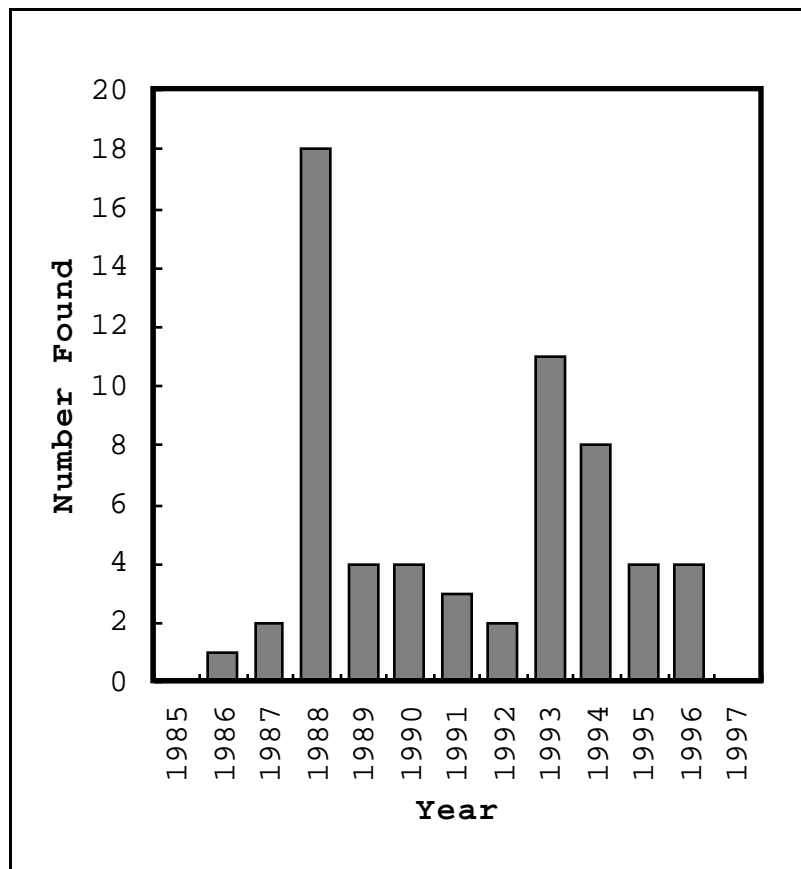


Figure 2. The number of new copper oxide superconductors discovered each year since their initial discovery in 1986. The second peak in the bimodal distribution in 1993 appears due to the introduction of the high temperature - high pressure synthetic method to the search for new materials. (courtesy R. J. Cava)

Two strategies for new materials discovery presently are operational in the field, which have proven successful in different research environments. In the chemistry-driven approach, research is concentrated on a group of reactions, compounds, or structural motifs which are believed to be interesting, or in need of development. In this research strategy the properties of the materials are secondary to the

discovery and structural and chemical understanding of the materials themselves. Such research programs are not only of high scientific value, but can also have a long-term impact on the course of applied research, when explored by experts in the context of their particular interests.

The second strategy for new materials discovery is the properties-driven approach. In this case, new compounds are sought which display a particular physical property or phenomenon. The motivation can be the exploration of a basic scientific issue, or the possible long-term technical application, or both. There is a whole spectrum of methods used in this approach, ranging from carrying out a few carefully planned experiments to executing a large number of wide ranging experiments (e.g. combinatorial chemistry). In these strategies, the finer points of chemistry are often secondary while properties are paramount - they are used in a feedback loop with the synthesis conditions to find the optimal material. This approach, although primarily properties directed, has often also led to significant scientific contributions in fundamental research. It can also stimulate the development of new synthetic methods when known methods are not up to the task.

The combination of both materials discovery strategies provides the basis for the advancements in the understanding of the complex relationships between composition, structure and properties that lie at the heart of solid state and materials chemistry.

Where we are going:

New materials play an essential role in fundamental scientific and technological progress in the physical sciences because their study frequently reveals new physical phenomena or forces re-evaluation of what has previously been thought to have been understood. This has been frequently demonstrated in the

past, often with dramatic consequences. A textbook example is furnished by the discovery of high temperature superconductivity. Table 2 shows a partial listing of new materials which have been discovered or studied extensively in the last 25 years.

Table 2: A partial list of new materials that have been discovered or extensively studied since 1973.

intercalation compounds	heavy fermion superconductors
fast ion conductors	microwave ferrites
charge density wave materials	metal hydrides
(Hg,Cd)Te	magnetic superconductors
Er-doped fiber amplifiers	III-IV semiconductors
incommensurate crystals	frustrated magnets
photorefractive memories	C ₆₀ , carbon nanotubes
non-linear optical materials	colossal magnetoresistance
organic superconductors	quaternary intermetallic superconductors
dilute magnetic semiconductors	small semiconductor clusters
spin glasses	GaN light emitting diodes
microporous solids	porous silicon
intermediate valence compounds	liquid crystals
metal-insulator transition compounds	polymer electrolytes
copper oxide, high T _c superconductors	quasicrystals

Casual inspection shows that the list is extensive and varied, and indicates that new materials discovery and research into their characterization has been very active and productive. It should be noted that new materials have been at the center of many thrusts in condensed matter science during this period. The rate of discovery remains very high, with new insights being furnished into many different areas of science through such

studies. This long-term trend, spanning two and a half decades, continues to this day, with no signs of slowing down.

Solid state and materials chemistry is increasingly regarded as an essential component of many multidisciplinary research programs. The rate-limiting step in many scientific studies in condensed matter physics, for example, is the availability of high quality materials. Further progress in solid state chemistry is envisioned through continuation of current activities and expansion in the following three areas:

1. New Synthetic Techniques. Scientific progress in solid state chemistry will likely be made both by research that focuses on purely scientific issues such as the development of new synthetic techniques, and by research which is aimed at solving long-term technological problems. Very few of the compounds which can be imagined have already been found, indicating the great potential for exploration of unknown areas, Figure 3. For example, only 0.01% of the possible quaternary intermetallic systems have been investigated. Maintenance of core expertise in previously established methods and concepts of solid state and materials chemistry is absolutely fundamental for the continuing discovery of new materials and the contribution of the field to the larger scientific community.

As has been repeatedly demonstrated, new materials can play an important role in fundamental scientific and technological progress and can be expected to continue to do so. The current development of materials of increased complexity should be expanded into new areas of research and development. *The continuing growth and vitality of the field requires that new avenues of research be taken into account as they arise.* Those new avenues constitute an important component of an overall program, as they may lead to unexpected findings whose applications or implications may only be appreciated in the future.

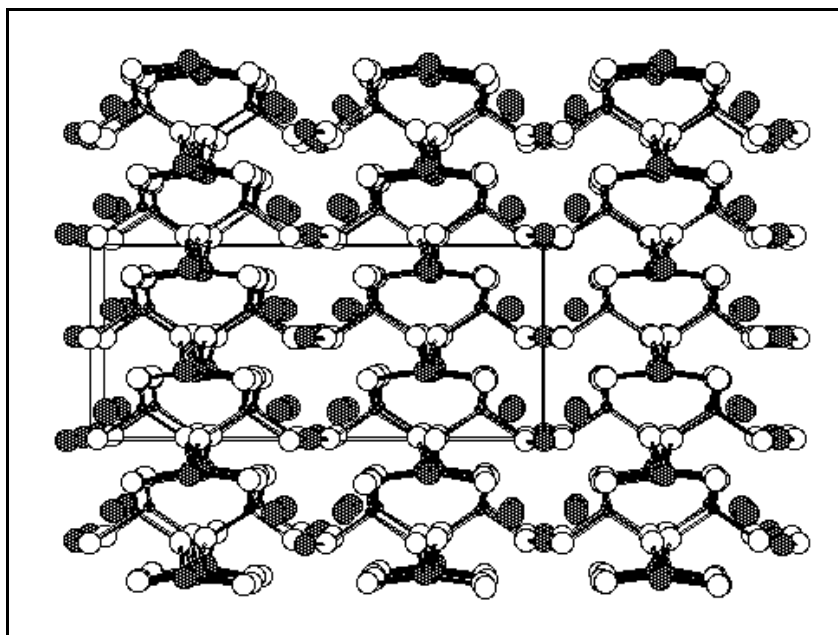


Figure 3. The new compound, $-K_2Hg_3(GeS_4)_2$, shown above, was discovered during a research program funded by the NSF whose purpose it was to investigate the potential of new synthetic methodologies. This compound, in a polar crystal structure, is highly transparent in the infrared, resistant to laser damage, and shows strong second harmonic generation. (courtesy M. G. Kanatzidis).

2. Multidisciplinary Research. The interdisciplinary nature of solid state and materials chemistry establishes expertise in areas outside traditional chemistry as an important component of successful research programs. Cognizance should be taken of the increasing impact of solid state and materials chemistry on the wider scientific community through an increase in interaction and communication with other disciplines. This theme is also stressed elsewhere in this document. To implement this goal, the participants in this topical presentation recommend increased multidisciplinary research and training of students through exposure to activities outside the usual chemical curriculum. This might occur through joint programs sponsored through the NSF, as is done, for example, in the focused research group program, where students and faculty

interact with others in different disciplines in specific research projects. Examples of such joint programs which could be established to involve interactions between solid state chemistry and condensed matter physics, solid state chemistry and electrical engineering and materials engineering, or solid state chemistry and biology. Students should be encouraged to broaden their interdisciplinary knowledge through the educational opportunities available in the relevant academic departments. Further, such multidisciplinary and collaborative research activities should be recognized as important in evaluation processes such as tenure decisions for young faculty.

3. Materials by Design. In an analogy with synthetic processes in organic chemistry, a long term goal in synthesis in solid state chemistry is to make materials by design: e.g. to make what is wanted instead of seeing what can be made. As part of this goal, reaction mechanisms need to be explored to help in determining reaction principles which will help direct the discovery of unknown materials. Further, as the understanding of structure-property relationships increases and computational methods become more accessible, it is expected that computer aided synthesis of new materials will play an increasing role, e.g., through prediction of crystal structures which has been stressed elsewhere in this Report. A more ambitious long term goal is to be able to predict the properties of complex materials from first principles. Just as X-ray diffraction in the past decade has become a tool which can be routinely used in small research programs without extensive crystallographic expertise, it would be of great utility if user-friendly theoretical modeling programs, such as those used in density functional theory, became available as a tool to be used by research groups in their synthesis programs. Such programs, for example, would be very helpful in understanding the electronic and magnetic properties of materials that have been synthesized.

Summary

The discovery, characterization and understanding of new materials is at the heart of solid state and materials chemistry. The new materials discovered by solid state and materials chemists play an essential role in both fundamental and applications oriented research in a broad range of scientific disciplines and technological systems. This has led to the rapidly growing recognition of solid state and materials chemistry in the past ten years as an essential component in multidisciplinary research programs- an indication of its vitality and emerging importance. Due to the complexities which naturally arise from the many-body interactions which occur in condensed matter, researchers are presently actively engaged in the process of discovering and developing the relationships between the compositions of materials and their structures, and at the same time, their structures and their physical properties. A wide variety of synthetic methods are presently being pursued in innovative ways to discover new materials. These methods generally either yield access to new regions of thermodynamic stability previously not available for synthesis, such as high temperatures and pressures, or access to kinetically stable phases synthesized at significantly lower temperatures and milder conditions. Further progress in solid state chemistry is envisioned through continuation of current activities and expansion in three areas: (a) consideration of materials of increasing complexity in new areas of research and development, especially by being inclusive of new avenues of synthetic research as they arise; (b) increasing the impact of solid state and materials chemistry in the wider scientific community through an increase in interaction and communication with other disciplines; and (c) pursuit of the long term goal of making materials by design through elucidation and understanding of reaction pathways, and increased theoretical guidance as part of the materials discovery process.

III. Hybrid Materials - M. D. Ward, Coordinator; T. Bein, G. Stucky, M. Tirrell, O. Yaghi.

The education of the next generation of materials scientists and engineers relies on conveying the fundamental principles underlying the design, synthesis, and properties of increasingly complex materials.

Numerous societal needs and the economic competitiveness of the US rely on the creation and manufacture of new materials with increasingly complex properties and function. It is becoming increasingly apparent that the materials needs of key sectors - Health, Environment, Education, Defense, Transportation, Energy, Advanced Technologies - are surpassing the capabilities of traditional single component, monofunctional materials. Consequently, it is inevitable that "hybrid materials", i.e., materials assembled from dissimilar and commonly incompatible components - generally for the purpose of achieving structure, properties and functions that cannot be realized with the individual components alone - will play an increasingly important role in future products generated by materials research and development.

Hybrid materials have multiple components that are organized into spatially identifiable domains with prescribed degrees of heterogeneity, on length scales ranging from nanometers to microns. The achievement of desirable properties and functions through integrated structures is already pervasive in the manufacturing and technology sectors: numerous familiar products can be described as hybrid materials (see Historical Perspective, below). Nevertheless, further advances are needed to meet applications requiring more complex functions, and to take advantage of designed synergistic interactions between the dissimilar components that introduce new properties or enhance product performance. Synergy can be important to produce desirable mechanical properties, optical properties, magnetism,

ionic conduction, selective adsorption and diffusion, catalysis, and charge transport. Hybrid materials may be the desired product, or may be process intermediates in which a hybrid architecture present during synthesis is required for achieving a material with desired structure, morphology, or properties. A key advantage of hybrid materials is their synthesis from "modular" components, which permit rational control and manipulation of property and function with unprecedented control. Multiple components provide more degrees of freedom in materials synthesis and promise much finer control over properties and function than is typically realized in simpler materials. Hybrid materials promise opportunities in cost reduction if inexpensive components can be combined to achieve materials with performance identical to, or even exceeding, more expensive alternatives. The flexibility provided by hybrid strategies may lead to alternative processing approaches that can be environmentally advantageous. Since hybrid materials often involve noncovalent bonding, at least during processing, unusual combinations of inorganic and organic materials can be produced in a compatible manner (e.g., nondegrading to the organic component). This vastly increases the toolkit available for materials synthesis. Softer forces during assembly may also permit repair of mistakes occurring during assembly.

In addition to multiple components, hybrid materials are characterized by structures of multiple length scales which can be tailored to fit the desired properties. In many cases, the smallest length scale is of small molecule dimensions, serving to trap or integrate a molecular or ionic species within a structure possessing order at a larger length scale. In many important examples of hybrid materials, the materials are multicomponent only *during* processing or synthesis; the multicomponent nature is used to template or mold in the controlled, larger length scale.

At some length scale, the character of hybrid materials as organized assemblies at multiple length scales, merges with the

character of devices and machines assembled to perform particular functions. When the features of devices and nanofabricated machines can be reduced to the ten nanometer level the concepts of hybrid materials and of devices tend to become indistinguishable.

An inescapable feature of *all* hybrid materials is the existence of interfaces. Consequently, *control* of interfaces and *their* properties is arguably one of the most important needs in the development of hybrid materials. Hybrid materials interfaces are exemplified by biological/microelectronic (e.g., protein/silicon); hard/soft (e.g., in lubricated surfaces); organic/inorganic (e.g., soft tissue/hard tissue; biomolecular ceramic composites, epitaxial organic films); and by porous/continuous (e.g., continuous frameworks or membranes with porous interiors). Interfaces separating dissimilar components may be as important as the components themselves with respect to materials properties, governing such phenomena as adhesion, friction, lubrication, permeability, electron transport, and stress transduction. This need to control interface properties implies that solid state chemistry must be attentive to new interface design principles and to functional molecular entities capable of straddling and stabilizing interfaces. Amphiphiles - molecules that possess two kinds of affinity within the same molecule - naturally straddle interfaces and can transmit stress and signals across boundaries between material elements. Recent advances in synthesis and characterization that make it possible to control interfaces and manipulate components at or near the molecular level indicate that the most significant advances in hybrid materials involve structure and property design at small length scales. These must be coupled through an understanding of how this translates into complex hierarchical structures defined by longer length scales.

The definition of hybrid materials presented here is intended to be broad and will undoubtedly continue to evolve with the development of complex materials. "Hybridicity" may

exist on macroscopic length scales or may pertain to well-defined dissimilar regions of a single molecule. Some workers may prefer to reserve this definition to describe materials with clearly defined regions of dissimilar components that can be detected by physical characterization methods. Alternatively, this term may be more powerful when used as a strategy, as a guide by which materials are designed. No matter how this is viewed, one may anticipate that hybrid materials will be key to future advances in materials research and products.

Historical Perspective of Hybrid Materials

Hybrid materials have played an essential role in all areas of society; an encyclopedic description of their contributions could would be an enormous undertaking. In the area of health biocompatible surfaces have been generated for medical implants of all kinds. These are necessary for the creation of non-thrombogenic interfaces for repair of the cardiovascular system. In some cases they play a key role both as processing intermediates and in the final product, as in the construction of porous scaffolds for bone growth and their subsequent interface with *in vivo* tissue. Hybrid materials are widely used as external health agents, as in ultraviolet sunscreen colloidal cremes (clays intercalated with organic dyes), controlled release pharmaceuticals, and wound treatment. Other biological substances that are hybrid materials based include mineralized composites (e.g., mother of pearl, decorative finishes, diatomaceous earth).

Almost every gallon of gasoline is the result of processing by synthetic zeolites and molecular sieves, which are porous materials assembled by condensation of an inorganic phase around a guest structure directing agent that may be a hydrated inorganic species or an organic molecule. Their use as catalysts, detergent builders (replacing less biocompatible phosphates), air (oxygen from nitrogen) separation, and nuclear waste cleanup agents is in the megaton range and continues to

grow. Commercially they are also used in other applications, including use as foaming agents for bulk items such as automobile steering wheels or packaging, which require intermediate temperature curing processes to create low density interiors and high density, high strength exteriors; water purification; dye encapsulation for enhanced lifetime and ease of dispersion; Carnot cycle air conditioning; and animal feed supplements.

One of the largest commercial applications of chemical assembly in current use, and being very actively further explored is the information industry, including computing, communication, measurement, and data storage. One of the most pervasive examples of self assembly in this class is high definition photographic film. In this case single sized silver atom clusters are assembled and organized in a three dimensional medium, with as highly ordered a three-dimensional periodic intercluster displacement as possible.

Computer chips consist of patterned semiconductor arrays, packaged with interconnects and low dielectric materials. The organic-organic and inorganic-inorganic interface chemistry of these composite structures must be defined at the angstrom level. The speed and capacity of these devices has increased at a phenomenal rate during the past five years, requiring increasing integration and multifunction incorporation at ever smaller length scales. The success of this effort has made this undertaking into one of the major economic engines of the United States economy for several reasons. First, research has shown that nanostructures functionally organized into coherent hierarchies will deliver both dramatically increased and/or new capabilities. Second, nanocircuitry has the potential to deliver a 10^9 enhancement in computing speed over present systems. This will require the creation of complex structures with approximately 5nm components. Third, at some point which is rapidly approaching, bottom-up chemical fabrication of hybrid based nanoelectronic devices will become not only economically

competitive, but might be the only economically feasible way to access components of dimensions less than 10 nm.

Numerous other everyday consumer products that have either their origins in or are hybrid materials include: non-stick cookware (Teflon with occluded heat-resistant coloring agents such as ultramarine - a small cage zeolite structure containing entrapped sulfur radicals); catalytic converters in automobiles which consist of ceramic porous monoliths of high surface areas and highly dispersed supported platinum clusters; organic-inorganic sol-gel films for hard coatings on windows and reflective surfaces; intercalation lithium ion batteries; exfoliated clay-polymer composites for the enhancement of strength and lifetime of commercial polymers; composite coatings for antireflectivity and antistatic properties; electrochromic displays; recording tapes; and even more ubiquitous, cement products.

Current Activities and Emerging Areas

In the following compilation increasing complexity serves as a guideline. Distinctions are made between systems constructed on pre-existing planar substrates (films), layered materials, and three-dimensional systems. Clusters are considered in the context of the resulting end product; for example, a layer of gold clusters would be considered a film. Obviously there are also different degrees of structural order associated with different materials; these range from crystalline to disordered. The 'hierarchy' or complexity of the materials is also of great interest; one could encounter unique or repeated (superstructure) sequences of components along different vectors of a reference frame, or 'nesting' of components, or smooth composition gradients.

1. Thin films

- Semiconductor quantum well heterostructures, such as laser diodes. Emerging area: blue laser diodes.
- Self-assembled monolayers such as thiols, tribology, adhesion, sensors. Emerging areas: photopatterned DNA films, cell adhesion, biosensors, sensor arrays; formation of patterned surface structures from block-copolymers.
- Epitaxial molecular films, self-assembled molecular (oriented) multilayers with alternating layers, organic/inorganic combinations such as phosphonates. Emerging areas: photovoltaics, barrier layers, nonlinear optical films, sensors.
- Self-assembled cluster layers and cluster/polymer multilayers. Emerging areas: gold cluster layers, surface enhanced Raman spectroscopy substrates, titanate sheets; applications: charge transfer, Coulomb blockade, and the like.
- Biomimetic growth of inorganic phases on organic layers. Emerging areas: semiconductor clusters, zeolites, shape selective chemical sensors.
- Hybrid sol-gel derived films, such as protective coatings, anti-reflection films. Emerging areas: molecular sieve membranes, sensors, biosensors.

2. Layered materials

- Layered metal phosphonates. Emerging areas: functional phosphonate materials: molecular sieving, catalysts, energy transfer, and the like.
- Modified layered structures by ion exchange, intercalation, condensations. Graphite intercalation. Exfoliation and re-assembly of layered materials. Ionic conductors such as -aluminas, catalyst supports. Emerging areas: fuel cell electrodes, new ionic conductors, pillared clays with tailored porosity and/or catalytic activity.
- Layered redox active hosts intercalated with polymers showing ionic and/or electronic conductivity. Emerging area: battery electrodes.

3. *Three-dimensional crystalline networks*

- Zeolites with organic structure-directing agents, and modified zeolites for separations and catalysis and ion exchangers. Emerging areas: transition metal containing zeolites, phosphors, chiral zeolites, stable ultra-large pore zeolites, chiral catalysts and separation materials, metal clusters and other clusters in zeolites, epoxidation catalysts, dyes in zeolites, sensors.
- Coordination and molecular networks involving organic molecules, metal ions or clusters connected by strong and/or weak bonding forces). Emerging areas: robust, porous networks with tailored porosity, highly specific molecular sieving/separations, gas storage, catalytic activity, nonlinear optical systems, drug forms with improved delivery behavior, and the like.
- Organic Ferromagnets and Conductors.

4. *Three-dimensional disordered networks*

- Sol-gel and polymer derived materials, including organic-inorganic hybrid materials. This is a vast area, with many opportunities to vary components and properties. For example, protective films, restricted reaction media, linked clusters such as silsesquioxanes with organic/organometallic bridges, stabilization of nanosize metal or metal oxide particles in polar matrices. Emerging areas: hetero-substituted silsesquioxanes as catalyst building blocks, optical dye inclusions for nonlinear optical applications, doped sol-gel materials and lens forms, encapsulated enzymes, novel magnetic materials, composites with exfoliated layered or porous materials, catalysts.
- Hybrid systems from mineralization in polymers. Emerging area: bioinspired composite formation.
- Mesoporous materials prepared in surfactant-directed syntheses. Emerging areas: mesoporous transition metal oxides, large-pore mesoporous materials with block copolymers, in situ modification of mesoporous materials with functional groups, control of three-dimensional macroscopic shape (spheres, oriented films, plates, and fibers, and self-organized shapes), bioseparations.
- Post-synthesis modified porous networks and mesoporous materials. Heterogeneous catalysts, chromatographic media. Emerging areas: grafting of functional groups

and metal complexes/clusters into mesoporous materials, stabilization of nanometer scale conducting wires.

- Lithographically sculpted/modified preformed bulk materials such as silicon which are 'hybrid materials' of highest complexity, electronic circuits. Emerging area: three-dimensional stacking of circuitry.

Synthesis and Processing

Simple atomic units

The general approach of building a material from components, ("building from the bottom up") resembles construction of a house from bricks and mortar. Using atoms, the direct deposition of atomic layers to create heterostructures is probably the most elemental approach to the construction of complex materials (atomic or molecular beam epitaxy for the production of semiconductor quantum well heterostructures provides numerous examples). This type of construction is closely related to chemical vapor deposition (CVD); deposition of components from the decomposition of specifically designed precursor molecules or reactants.

Molecular units

The next type of building blocks of increasing complexity involve molecules (mostly soluble) such as alkyl thiols for the construction of self-assembled layers on metal substrates, the vast number of coordination networks (metal ions or clusters connected by network-forming ligands), and molecular crystals that have distinct components assembled in new arrangements. Molecular properties are being transferred (and modified) in the resulting solid.

Assembly with formation of bonds between building blocks

The assembly process becomes more complex if strong covalent bonds are formed between some components of the system. The vast field of sol-gel chemistry (including organic-inorganic hybrid materials) provides numerous examples, both in thin films

and bulk forms. Other families of systems include zeolites with organic structure-directing agents, layered metal phosphonates, and mesoporous materials prepared in surfactant-directed syntheses.

Giant building blocks (relative to typical molecular size) are now being created using the principles of colloid chemistry. In this approach, components that have their own extended lattices are being assembled into disordered hybrid materials or even superlattices. Sometimes, these building blocks are combined with polymeric, 'soft' components. On planar substrates, examples include the formation of layers of stabilized gold clusters, or the assembly of exfoliated titanate sheets with polyelectrolytes. Extended networks include sol-gel embedded iron clusters, or superlattices of stabilized nanometer-size CdSe clusters.

Modification of existing structures

A rather different synthetic approach is the modification of existing extended structures by ion exchange, intercalation, or condensation (some examples of "*chimie douce*"), in order to form new hybrid materials. Graphite intercalation is probably the archetype reaction in this family.

Sculpting of pre-formed materials

Finally, lithographic 'sculpting' of preformed bulk materials such as silicon has been the basis of the microelectronics industry. A vast arsenal of etching and thin film deposition techniques can be used to produce an immense variety of 'hybrid materials' of highest complexity: electronic circuits.

Forces used in the assembly of hybrid materials

In the construction of many hybrid materials, non-covalent forces (often hydrogen bonding) are utilized to assemble an enormous variety of molecules and components into more complex structures. Often structural control derives from the ability

to arrange hydrogen bond donors and acceptors on the building block molecules with synthetic methods of organic chemistry.

The formation of a specific covalently bonded structure can be assisted by weaker forces: examples range from construction of self-assembled mono- and multilayers with various functionalities (using covalent bonds for attachment, and dispersion forces that help assemble the film structure) to zeolite synthesis with organic 'templates'. Other examples include multilayers of charged components such as polyelectrolytes (adding electrostatic forces), the intercalation in pre-assembled layered hosts (sometimes using electron transfer), construction of chelate complexes in nanoscale zeolite cages (size-entrapment), and the intriguing structural control obtained in the liquid crystalline assemblies used for the synthesis of metal oxide mesostructures. The coordinative bond (local bonding geometry of transition metal ions) can also be used when assembling building blocks in three dimensions, for instance in coordination polymers linking transition metal sites with appropriate ligands.

One of the most powerful concepts in the synthesis of complex solids is the "template" approach. Often an organic molecule is used to impart certain structural features to the solid under construction. Many examples pertain to the synthesis of zeolites, but more recently, the structure of some coordination polymers has also been modified by using organic structure directors or solvents. The non-covalent interactions can exert exquisite control over the structure of the resulting system. For example, the new family of mesoporous materials is formed in a cooperative assembly process from organic surfactants and inorganic building blocks that crosslink during synthesis. The template concept can also be turned around to use hollow hosts as templates for the stabilization of guests in certain shapes, such as metal wires, clusters, etc.

Often, the interfaces generated in (or used in the generation of) the hybrid systems define their structure and properties. This can range from structure-directing in zeolite synthesis to the wetting behavior of perfluorinated self-assembled monolayers. The common principle in most, if not all, of these hybrid systems is that they are far from thermodynamic equilibrium. They exist because they are prepared under low-temperature conditions that favor metastability. This feature creates some intriguing similarities with biological objects (composites in bones, shells or tissues are very complex hybrid systems).

There appear to be no limits to the creation of novel hybrid materials - the vast number of building blocks and assembly concepts continues to be developed further, and their potential combinations are virtually infinite. Numerous physical properties and potential applications of hybrid materials are now being explored, including structural, non-linear optical, magnetic, and electronic effects, as well as many catalytic reactions.

Education

This topic is being extensively covered elsewhere in this Report. Nevertheless, it is appropriate to discuss this matter briefly in the context of the current presentation. The education of the next generation of materials scientists and engineers relies on conveying the fundamental principles underlying the design, synthesis, and properties of increasingly complex materials. This will require an interdisciplinary approach to education, so as to increase the breadth of students, without, however, sacrificing depth. This is a critical challenge that argues for a substantial revision of the curriculum, or of programmatic requirements. At the very least, new scientists must become sufficiently exposed to multiple facets of materials - chemistry, physics, solid state structure - so that communications between different disciplines is

facilitated, thus permitting individual scientists to feel comfortable in areas in which he or she has had no formal training.

Characterization

This topic is also being covered in other sections; we concentrate on aspects specific to hybrid materials. The synthesis and utilization of hybrid materials have undergone recent explosive growth, as have techniques for controlling the chemistry and structure of interfaces. In the same span of time new characterization tools, such as scanning probe microscopy, have been invented, and have been invaluable in characterizing microscopic structure. However, their development has not kept pace with problems posed by this growing class of new materials. In general, hybrid materials have structures on many length scales, are complex in composition, and assemble via incompletely understood dynamical processes involving both strong and weak forces. The increasing importance of hybrid materials is likely to drive the development of new tools for imaging and determining structure on several length scales, for measuring materials properties with better spatial and temporal resolution, and for understanding dynamical processes, structure, and properties on a theoretical basis.

The following are perceived as important current needs in hybrid materials characterization and analysis:

- *Determination of structure on several length scales.* Single crystal and powder diffraction methods are arguably the most important characterization tools in solid state chemistry. Hybrid materials, however, are often multi-phase or amorphous. Even when one crystalline phase dominates most of the material (for example, in a colloidal crystal made from semiconductor nanocrystals), there are important issues of size dispersity in the building blocks, epitaxy and degree of order, and hierarchical structure. The accurate determination of domain

and particle sizes in this class of materials is problematic, and improved scattering, imaging, and spectroscopic methods are needed. Information-rich, spatially localized spectroscopies, such as multiphoton, confocal, and near-field optical techniques, are likely to be increasingly applied to hybrid materials problems in the future. Solid-state NMR is also continuing to develop as a tool for determining local structure and connectivity in solids. In all these areas, there is a strong need for both theoretical and instrumental development.

With thin films and nanoscale materials, scattering and spectroscopic methods will become increasingly useful as the brightness of sources (neutron, x-ray, lasers) and the sensitivity of detectors increases. The same developments are likely to lead to new imaging and topographic methods, using particles and short-wavelength radiation. There are also opportunities with this class of materials for combining characterization techniques in new ways: for example, combining rheometry and scattering methods to determine particle size distributions.

- *In-situ structural methods, imaging, and spectroscopy.* The synthesis of materials that have structures on several length scales implies complex reaction mechanisms, as well as parallels with the formation of hierarchical structure in biological systems. So far, the principles underlying these reactions are poorly understood and thus present an important fundamental challenge. Developing a conceptual and theoretical framework for these reaction mechanisms requires *in-situ* methods that work across several length and time scales.

- *Buried interfaces.* Interfaces are an inherent component of hybrid materials and thin films. There is an increasing need for non-destructive, sensitive techniques to probe the detailed structure and properties of buried interfaces within hybrid materials. At present, relatively few probes exist that are specifically sensitive to these interfaces (an exception, in

the case of contacting isotropic phases, is second harmonic generation). The development of new interface-specific methods is therefore an important opportunity area.

- *Defects and trace components.* Often structural defects, impurities, and trace components have an extremely important influence on the macroscopic properties of materials. The electronic properties of doped semiconductors are perhaps the most familiar example of this effect. Many examples also exist within the realm of hybrid and composite materials. For example, the ferroic properties of oxide ceramics are influenced by very low concentrations of hydroxyl defects. Likewise, the mechanical strength of sea urchin spines is a consequence of very small amounts of protein inclusions in a calcite single crystal. The secondary structure of the protein that is responsible for its biological function is only stable within the calcite crystal. Both examples contain a minority component that must be characterized *in situ*, in order to understand its effect on the properties of the composite. These problems suggest the need for new developments in structural analysis that yield information on small amounts of localized impurities or defects in hybrid materials.

- *Theoretical development and computational tools.* There is a need for theoretical development at several levels. It is widely appreciated that the synthesis and properties of several kinds of hybrid materials (for example, porous solids, polymer-crystal composites, and colloidal crystals) involve weak, long-range forces acting in concert with strong short-range forces. The measurement of these forces, molecular-level characterization of interfaces, reaction mechanism studies, and determination of phase equilibria are important experimental challenges. These studies create new, interesting, and difficult problems for theorists. Accurate simulations of these phenomena presently range from the expensive to the impossible, because they involve a wide dispersion of length and time scales. The development of computational methods and tools is

needed to tackle this problem, to guide measurements, and to assist in the interpretation of experimental data (for example, in experiments aimed at measuring local forces). The synthesis of hybrid materials is rational in a sense, but at present is guided only by heuristic rules, and the products are often totally unexpected. This situation could be improved by a better theoretical understanding of the chemistry of interfaces (e.g., the surfactant-inorganic interface in porous materials synthesis), phase equilibria, and reaction mechanisms.

Challenges and Future/Emerging Needs

The future needs for hybrid materials are apparent in key sectors of the economy as well as areas of importance to society, including Health, Environment, Education, Defense, and Technology and Competitiveness. The advancement of these materials hinges on several key challenges with respect to elucidating fundamental scientific principles, developing synthetic strategies, and materials design.

Challenges

Fundamentals

- Establishing structure-property relationships that transcend length scales
- Elucidating the role of weak non-covalent forces on assembly, including molecular organization at interfaces
- Developing new principles for the control of interface and three-dimensional structure
- Providing new computational tools for prediction and design of properties that facilitate the elucidation of structure-property relationships and provide guidance for synthesis
- Setting up new methods for rapid development of new materials and optimization of properties and function, as discussed elsewhere in this report in further detail

Synthesis

- Synthesizing new materials that exceed existing performance and durability by tenfold, while reducing cost
- Introducing multiple levels of functionality
- Establishing the degree of robustness of different materials and interfaces, during use and in synthesis/processing
- Establishing structure control at the molecular or near-molecular level
- Exploiting higher dimensional networks for materials synthesis
- Developing protocols for using self-assembling films that can be prepared at lower cost under ambient conditions
- Setting up gradient structures

Performance

- multifunctional
- reproducibility
- gradient structures
- specific molecular recognition
- durability and cost
- prescribed mechanical properties

Some future products

- shape selective chemical sensors
- quantized particles by suitable sizing
- morphologically controlled microstructures
- encapsulated molecular wires and redox storage systems
- bioinspired composites
- improved drug delivery systems
- stable porous zeolite and molecular frameworks
- nanoporous media designed for molecular separations
- new optical materials (e.g., gradient structures)
- environmental remediation
- tissue engineering and physiological interfaces
- highly specific, controllable separations
- modular catalyst systems
- responsive materials

**IV. Societal Needs and Technological Opportunities -
D. W. Murphy, Coordinator; A. Sleight, T. Vanderah,
S. Whittingham.**

It is important both to sustain the exponential growth of existing technology and to encourage discontinuous breakthroughs. This requires a portfolio of research activities that are insulated from technology to the extent that adventurous paths are pursued, but not isolated from the major technological driving forces.

The primary goal of solid state and materials chemistry research is to ensure that the necessary fundamental knowledge base exists for emerging and future materials related technologies. That knowledge base encompasses the generation of materials, the relationship of their properties to structure and processing, and the techniques to evaluate relevant structures, properties, and analyses. The application of that knowledge base to technology depends on strong interactions between the research and application communities.

Materials have had a strong impact on technology and have often led the way in new technologies. Listed below in Table 3 are examples of general ways that materials chemistry impacts topics identifiable to the public.

Societal Needs and Technological Opportunities

The primary goal of solid state and materials chemistry research is to ensure that the necessary fundamental knowledge base exists for emerging and future materials related technologies. That knowledge base encompasses the generation of materials, the relationship of their properties to structure and processing, and the techniques to evaluate relevant structures, properties, and analyses. It can be argued that the grand challenge is to understand, control, and predict the structures

and properties of solids so as to generate new materials with superior physical properties.

Table 3. Identifiable public topics and impact of materials.

Health

diagnostic tools, biocompatible materials...

Energy

production, conversion, storage, efficiency...

Environment

energy efficiency, sequestration, insulation, sensors...

**Electronics and
Communications**

information storage, displays, packaging...

Transportation

sensors, energy conversion, structural...

Security

national, airport, personal...

Science

gems and minerology, biomimetic, reaction mechanisms...

Education

train future scientists, help society become more technologically literate and capable...

Advances in materials have been a large factor in improving both the quality of life and quantitative (e.g., Gross National Product) measures of it. The list above in Table 3 provides specific examples of general ways that materials chemistry impacts our everyday life.

History has repeatedly demonstrated that progress is made through both sudden bursts of insight and by logical extension of current technology. The semiconductor industry is a good example of both modes. In the early 1960's it was not at all obvious that integrated circuits beyond a few transistors would be viable; yet for the last two decades growth has been very predictable following Moore's Law: Technologies dependent on the knowledge base generated by Solid State Chemistry and Materials are growing as fast as 50% per year; to continue this trend requires a steady stream of Solid State Chemistry and Materials research to support present technology and to seed new technologies. Moore's law has been extremely accurate in predicting a variety of quantities such as information storage density, the cost of a transistor, or the number of transistors per unit area over two decades. The law does not prescribe how to achieve such results - only that it will happen. Getting there requires innovation and leads researchers to ask questions such as how to make a transistor for a picodollar, or where the current manufacturing process breaks down, or what other materials or phenomena could provide a new paradigm. The law serves as the basis for a roadmap for the chemically based industries. Many other industries have or are embracing roadmaps which are primarily used for business planning, but can help researchers identify appropriate areas of research. The importance and scope of materials chemistry evolves and grows in response to the emerging technological needs and opportunities.

It is important both to sustain the exponential growth of existing technology and to encourage discontinuous breakthroughs. This requires a portfolio of research activities that are insulated from technology to the extent that

adventurous paths are pursued, but not isolated from the major technological driving forces (such as massive computational power, a greater emphasis on environmental impact, portability of communications, etc.). The portfolio requires allocation of resources to the broad areas of knowledge which those technologies must draw on (examples include surfaces, defects, optics, high frequency behavior, etc.) and to the skill sets that will be needed to obtain this knowledge (theory, analytical techniques, materials preparation, etc.). At the same time, the portfolio must include activities that stimulate other scientists and may lead to new technologies.

The U.S. ranks very highly in the world's best overall materials research portfolios, thanks to strong government support, strong research universities, and a healthy industrial base. Historically, the U.S. solid state community has been known for its strong leadership in structure-property relationships, even though research outside the U.S., particularly in Europe, has dominated the initial discovery and structures of new solid state inorganic compounds. While we need to maintain our historical strength, a stronger presence in the generation of new materials is critical because the rest of the world has followed the US lead in placing greater emphasis on structure-property relationships. While in previous decades one was able to scour the literature for materials whose important properties had been ignored, such knowledge will increasingly be claimed by the initial discoverer. Another danger signal on the horizon derives from the significant scaling back of research in the industrial sector. This group of researchers provide the key conduit for information exchange between industry and academia. Mechanisms to nurture those connections should be encouraged. Mechanisms such as Cooperative Research and Development Agreements exist, but reviews are mixed, due to issues of intellectual property which often limit complete idea sharing and dissemination of results. Sabbatical leaves for academics in industrial laboratories, and

tutorial workshops at various national and regional scientific meetings are other possibilities.

Table 4 on page 51 lists some accomplishments and opportunities in the solid state chemistry and materials community, aligned with publicly identifiable topics. These examples are illustrative and not meant to be complete or exclusive. It is highly satisfying that the interdisciplinary nature of the subjects indicates that many of the accomplishments in the area of solid state chemistry and materials are shared with other disciplines.

Table 4. Accomplishments and opportunities in solid state chemistry and materials.

<u>Health</u>	<u>Energy</u>	<u>Environment</u>	<u>Electronics / Communications</u>
Piezoelectrics for ultrasound diagnostics	High energy-density batteries	Waste encapsulation and disposal	Displays (phosphors, liquid crystals)
Soft contact lenses	Photovoltaics	Oxygen sensors	Dielectric materials
Pacemaker batteries	Thermoelectrics	Catalytic converters	High resolution displays
Drug delivery	Nafion membranes for fuel cells	Alternatives to toxic materials	Polyamide interlayer dielectrics
X-ray phosphors	Catalysis	Mineral processing waste reduction	Packaging semiconductor components
Liquid crystal thermometers	Intercalation batteries	Freon-free refrigeration	Lasers and frequency doubling
MRI coils	Solid oxide fuel cells	Solid acids	Piezoelectric filters / resonators
<i>in vitro</i> sensors	Reversible O ₂ electrodes	Super insulation	Optical fibers and amplifiers
			Indium-free transparent conductors
			Photoresists
<u>Transportation</u>	<u>Science</u>	<u>Education</u>	
Plastics to replace metals	Pore-size control in silicas	ICE program and materials teaching companion	Storage media - optical and magnetic
Stronger/lighter structural materials	High-T _c superconductors	Internet courses for continuing education in materials	High and low-dielectric materials
Corrosion-resistant materials	Solid state reaction mechanisms	Interdisciplinary training and communication	High Q, frequency filters
Corrosion protection	Negative thermal expansion materials	American Chemical Society materials chemistry exams	
Pollution-free vehicals - hybrids	Combinatorial materials discovery		<u>Security</u>
Actuators	Biomemetic materials		Night vision and infrared detectors
Smart mirrors	Fullerenes		Transportation security systems
Nd ₂ Fe ₁₄ B magnets			Sonar detectors
Catalytic coverters			Bullet-proof vests
Oxygen sensors			Explosives detectors

PANEL DISCUSSION REPORTS

**V. Panel on Education - S. M. Kauzlarich, Coordinator;
J. Chan, A. Ellis, M. Geselbracht, B. Reisner,
A. Stacy.**

Solid state and materials chemistry is an interdisciplinary science essential to progress in science and technology. Providing a skilled, diverse work force for this field, and developing an appreciation for the uniqueness of solid state chemistry among students and the public is only achievable through advances in education.

This panel considered the general topic of education in the broad context of both solid state chemistry and materials chemistry as a unit, since both the educational problems and the opportunities in these two disciplines are very closely linked.

Solid state and materials chemistry is an interdisciplinary science essential to progress in science and technology. Providing a skilled, diverse work force for this field, and developing an appreciation of the uniqueness of solid state chemistry among students and the public is only achievable through advances in education. We treat education in this area in the broadest sense, and consider the different levels of education that need to be addressed. The present section is organized according to different target audiences, which have been categorized in four groups: students, colleagues, the practitioners of solid state and materials chemistry, and the public.

What are the issues?

- Students The influx of new faculty in solid state and materials chemistry presents an unprecedented opportunity to introduce students to the chemistry of extended structures, alongside the chemistry of discrete

molecules. However, there are still many institutions where students graduate from chemistry departments never having been introduced to extended structures. This raises issues for education and training at several different levels. First, at a general level, science literacy for all students should include an introduction to and appreciation of materials. This requires the introduction of solid state and materials chemistry to K-12 students and its continued presence throughout the undergraduate and graduate curriculum. Second, to enrich this field it is necessary to increase the number, quality, and diversity of students that we attract. This requires focusing on introductory chemistry courses, as these are the pressure points or gateways for the rest of the chemistry curriculum. A background in solid state and materials chemistry will enhance the capabilities of incoming graduate students who will specialize in this area.

- Colleagues It is necessary to educate faculty colleagues to the importance of integrating materials topics in the chemistry curriculum, regardless of their own research interests. Colleagues should be educated and encouraged to gain a better appreciation for the role of chemistry in materials research. A better understanding not only impacts the hiring and tenure decisions for new faculty in solid state and materials chemistry, but also the allocation of resources, particularly at the departmental level.
- Practitioners Educating ourselves about opportunities and innovations both in research and teaching serves to inform and unite the solid state and materials chemistry community. For example, sharing information on available resources and expertise strengthens the research capabilities of the community. It is essential for scientists in this field to avoid working in isolation;

rather, they should share and create new ideas in education as a community.

- Public It is necessary to ensure a more visible integration of solid state and materials chemistry in public presentations of chemistry topics. This is achievable only through the successful education of the three groups discussed above. Direct public outreach that highlights the chemistry in technological products could help improve the public perception of the value of chemistry and chemists.

What is the current status?

Pre-college Level. NSF funding supports projects aimed at pre-college teachers and/or students through the Directorate of Education and Human Resources at the following website: (<http://www.nsf.gov/home/ehr/start.htm>). At the K-6 level, many of the projects cross a number of disciplines such as physical sciences, rather than falling within a single discipline such as chemistry. At the high school level, some projects are separated into chemistry, biology, and physics, but are generally not as specific as solid state, materials chemistry, or materials science. Many projects may include a materials science component, but may not include those words in their description. By polling faculty, networking, searching the NSF database and searching the Web, the panel was able to identify the following projects that directly relate to materials and thus, to solid state and materials chemistry.

- Explorations of Materials Science, a module developed by General Atomics¹ that includes investigations of a metal, polymer, and ceramic.
- Superscience, a collection of K-6 enrichment activities. Some of the physical science components of modules developed for Full Option Science Systems (FOSS; Lawrence Hall of Science, UC-Berkeley), and Science and Technology for Children (STC) are materials-science related. These projects include

investigations with solar cells, advanced magnetic materials, NiTi memory metal, superconductors and slime.

- All of the NSF-funded Science and Technology Centers (STC)'s as well as the Materials Research Science and Engineering Centers (MRSEC)'s have an education component.² Most of the programs maintain an active website³ detailing their outreach activities aimed towards their community. Many of these centers also provide training, hands-on-activities, student materials, and teacher aids for educators, in order to disseminate and encourage the inclusion of materials as part of the K-12 curriculum. One example is the Materials World Modules Program (see the web site at <http://mrcemis.ms.nwu.edu/mwm/index.html>); a module is available on composites, and additional projects are currently being field tested.

College Level. There are several different approaches for providing solid state and materials chemistry education to students at the college level: through formal course work, through special programs in solid state and materials chemistry, and through undergraduate research opportunities. The current status of projects receiving NSF funding in these area are very promising. The presence of solid state and materials chemistry in curriculum development projects was assessed by a survey of projects funded through the Division of Undergraduate Education (DUE). A list of 44 proposals was generated, using the NSF database for projects funded since 1994 that contained the words 'materials science' or 'materials chemistry'. Education at the college level is now an integral part of all research based proposals which involved solid state and materials chemistry. In addition, the educational components of STC's and MRSEC's mentioned above impact many undergraduates. Undergraduate research opportunities in solid state and materials chemistry are currently funded through individual principal investigator awards, as well as by Research Experience for Undergraduates programs. The Summer Research Program in Solid State Chemistry for Undergraduate Students and College Faculty (<http://www.usc.edu/dept/chemistry/nsfsumprgm/>) deserves

particular mention as being highly successful. This program has been in place since 1985 and has hosted approximately 20 students and 5 faculty per year. This adds up to a total of 240 students and 60 faculty since its inception. The participants involved approximately 40% women and 15% minorities. Figures through 1996 show that 52% of the participants pursued graduate education in chemistry, with an additional 16% going into graduate programs in related fields such as materials science, engineering, and biochemistry.

It is more difficult to assess the current status of formal course work in solid state and materials chemistry. A Web-based survey of 57 of the top funded (total research dollars and/or total NSF funding, FY94) chemistry departments was conducted: more than 90% of these schools include some mention of solids and materials in their course offerings.⁴ However, at the undergraduate level, the representation of solid state and materials chemistry in the curriculum ranged from a topical course to a few lectures in general chemistry. A more comprehensive presence of solid state and materials chemistry throughout the curriculum is encountered at institutions with faculty members whose research interests are in this general field.

Several recent and ongoing projects serve as excellent models for incorporating solid state and materials chemistry into introductory chemistry courses. Materials-intensive general chemistry courses have been developed by Gary Wnek and Peter Ficalora at the Rensselaer Polytechnic Institute (G. E. Wnek and P. J. Ficalora, *Chemtech*, **1991**, 21, 664) and by M. Stanley Whittingham at SUNY-Binghamton (see the site at <http://imr.chem.binghamton.edu/>). Engineering students at RPI take two semesters of the "Chemistry of Materials" course that was initiated in 1988. The course is jointly taught by faculty in chemistry and materials science and engineering. Wnek has launched a version of "Chem Materials" at Virginia Commonwealth University in 1997, co-taught with faculty affiliated with the

chemistry department. Virginia Commonwealth is also in the process of planning a jointly taught (chemistry and chemical engineering) organic chemistry sequence, bringing in industrial chemistry; an applied inorganic chemistry course for juniors is in the discussion stage, which would also be jointly taught and which would span some established (sulfuric acid manufacturing) and new (microelectronics fabrication) inorganic chemistry. Wnek is working on a textbook based on this course with a colleague, Mark Palmer.

A variety of instructional materials has been developed by the Ad Hoc Committee for Solid-State Instructional Materials (supported by NSF, Dreyfus Foundation, and the American Chemical Society), in response to the "Report on the National Science Foundation Undergraduate Curriculum Development Workshop on Materials," (Oct. 11-13, 1989); National Science Foundation, Washington, D.C., April 1990. This report highlighted the need to integrate solids into introductory chemistry and physics courses by providing compelling solid-state examples for core concepts. The effort is summarized in the following articles: "Materials Chemistry. An Emerging Discipline," L. V. Interrante, L. A. Casper, A. B. Ellis, Eds., *Adv. Chem. Ser.* **1995**, 245, ACS Books, Ch. 2; "You Do Teach Atoms, Don't You? A Case Study in Breaking Science Curriculum Gridlock," L. Lyons and S. B. Millar, University of Wisconsin-Madison LEAD Center, 1995; A. B. Ellis, *Chemtech*, **1995**, 25, 15, and *J. Chem. Ed.* **1997**, 74, 1033. A number of products have been generated from this project,⁵ including a model kit for solid state structures. ICE (Institute for Chemical Education) has sold over 1000 of these kits to date. An example of a one-semester introduction to chemistry for science and engineering majors in which these new instructional materials are integrated is given at the following website:

(<http://genchem.chem.wisc.edu/genchem/FALL97/109/Ellis/ellis.htm>)

Much of this material has also been used in the two-semester nonmajors course sequence at the University of Wisconsin-Madison.

Other perspectives on materials education, including polymers and materials science, are important in the education of students. In our course survey, only information on courses within chemistry departments is provided. However, the panel recognizes that education in the area of polymers and materials sciences benefits both students and faculty and is a valuable resource. A few highlights of educational activities in these related disciplines are presented here. In the area of polymers, there is the POLYED project, the American Chemical Society polymer education effort at the University of Wisconsin-Stevens Point, under the direction of John Droske, which has many instructional materials available. POLYED also sponsors scholarships for undergraduates in polymer science. Examples of the Materials Science perspective can be found in the following articles:

- (1) "Materials in the Undergraduate Chemistry Curriculum" S. Whittingham, *Materials Research Society Bulletin* **1990**, 15, 40.
- (2) "The Computer as a Materials Science Benchmark," D. J. Campbell, J. K. Lorenz, A. B. Ellis, T. F. Kuech, G. C. Lisensky, S. Whittingham, *J. Chem. Ed.* **1998**, 75, 297 (American Chemical Society). This article is featured as part of the 75th anniversary volume of *J. Chem. Ed.* The use of various materials in a computer illustrate the rapid development of materials science over the past 50 years; in addition there is speculation on where the field may be headed in the next 25 years.
- (3) The August 1990 volume of the *Materials Research Society Bulletin* addresses many areas of education.
- (4) "The Introduction of Materials Science into the Chemistry Curriculum and Chemistry into the Engineering Curriculum," W. Gloffke, and T. Kotch *Proceedings of the American Society for Engineering Education* **1990**, 897.

Through the American Chemical Society Committee on Professional Training, chemistry departments can provide an option to chemistry majors who wish to enhance their background in materials or in polymers. Currently, the American Chemical Society web page indicates only one institution which features this option for materials (the U.S. Air Force Academy). Ten institutions have such an option in the polymers area. (By contrast, 74 institutions have a biochemistry option). SUNY Binghamton has also adopted this option. Details on the process required to institute these programs can be obtained through the ACS web site (<http://www.acs.org/cpt/hp.htm>).

Graduate School Level. The NSF has instituted a new program called Integrated Graduate Education in Research and Training (IGERT):

(<http://www.nsf.gov/home/crssprgm/igert/start.htm>)

which will replace of the Graduate Research Traineeship (GRT) program. The program will emphasize multidisciplinary projects and as such is a natural avenue for furthering solid state and materials education at the graduate level. Out of 62 full proposals that were reviewed, approximately 8-10 are materials related; NSF plans to fund approximately 20. The University of Houston offers a Certificate in Materials Science to graduate students. It does not have a separate department in Material Science and Engineering. This program provides students with the interdisciplinary training necessary to work in solid state and materials chemistry. An example of distance learning is the new online MS program in materials at SUNY Binghamton.

Where are we going?

Recommendations to the community. We offer specific recommendations to improve the current level of education and the educational outreach at all levels. These recommendations

are aimed at providing education to the larger materials community and are inclusive rather than exclusive of the subdisciplines within materials research. We also suggest ways to increase the degree of cooperation at the national level, which will also impact the local level.

Guidance to students:

1. Encourage the integration of solid state and materials chemistry into the undergraduate chemistry curriculum by the following mechanisms:

- Hold workshops for textbook authors and publishers to facilitate the incorporation of materials into traditional chemistry texts.
- Create comprehensive solid state and materials chemistry textbooks that provide a fundamental framework for a core curriculum.
- Encourage the establishment of the American Chemical Society-certified Materials Chemistry option for bachelor level degrees at more institutions.
- Team teach a materials course with faculty from polymers, materials science, or other related discipline.
- Establish a Ph.D. in Chemistry with emphasis on Materials Science.
- Develop a new paradigm for undergraduate research in solid state and materials chemistry.

One way that the community can assume a leadership role in chemistry education is by developing an innovative course to introduce students to solid state and materials chemistry which is not merely an add-on to the current chemistry curriculum. Instead, we propose to engage groups of students in research on a specific topic in solid state and materials chemistry over the course of approximately two years. The course would be offered

as a one unit course (per semester) that integrates other courses that students are taking, thereby encouraging them to apply the concepts introduced in the standard chemistry courses to interesting and challenging problems in solid state and materials chemistry. This is a new approach to engaging undergraduate students in research, by encouraging them to work cooperatively with focused guidance from faculty. We envision that several faculty would propose jointly a specific research topic to the students and then serve as their advisors. Ideally, the faculty would be at several different campuses and include departments other than chemistry. Each time the course is offered, the research topic could change. This would provide a new model for engaging students in research, for informing them of opportunities at the frontiers of research in solid state and materials chemistry, and for strengthening interactions within the community, both across disciplines and across campuses. We propose to call the course: "Structured Adventures in Solid State and Materials Chemistry."

2. Facilitate communication from NSF-sponsored programs with an educational component (CAREER, MRSEC, STC, IGERT) to the larger chemistry community, in particular:

- Provide links to existing chemistry education efforts, such as the major NSF-funded consortia pursuing systematic reforms in the undergraduate chemistry curriculum.
- Establish mechanisms for widely distributing the results of educational innovations in solid state and materials chemistry to the wider chemistry community.

Guidance to our colleagues and ourselves:

- Ensure a solid state and materials chemistry presence in symposia at American Chemical Society, Materials Research Society, and American Physical Society meetings.

- Provide opportunities for tutorials and plenary lectures in cutting-edge areas of solid state and materials chemistry.
- Develop and maintain a Web site for the solid state and materials chemistry community that informs and cultivates opportunities, ideas, and innovations. Some of the specific links recommended from the panel include:

1. Teaching resources. This would include links to useful web sites for teaching and learning solid state and materials chemistry as well as model examples of the incorporation of this discipline into the chemistry curriculum.⁶

2. A list of faculty homepages in the solid state and materials community. This should be especially useful for prospective undergraduate students looking for graduate programs in solid state and materials chemistry.

3. Semester, summer, and co-op research opportunities for undergraduates such as Research Experience for Undergraduates sites with a solid state and materials component, the NSF summer solid state chemistry program, and the SERS fellowships at Department of Energy laboratories.

4. Opportunities for research interactions between members of the academic community and of the national laboratories.

Guidance to the Public

- The solid state and materials chemistry community should write articles about solid state and materials chemistry that reach the general public in venues such as magazines and newspapers.
- Participate in the dissemination of materials by connecting to existing programs.
- Be involved with schools in the community to make a difference at the local level.

The community has made a good start in educating all the groups mentioned above, but there is still much more to be done. There are opportunities for more involvement of faculty and scientists in the education of the public. We urge the NSF to continue to play a major role in providing opportunities for growth in educational programs at all levels.

References in the text may be found in Appendix B on page 78 of this report.

Acknowledgments. We thank a number of individuals who have provided essential information and resources. In particular, we are grateful to the Program Directors of the Division of Undergraduate Education: Frank Settle, Susan Hixson, and Peggie Weeks for information, resources and provocative discussions. We are also thankful to Wyn Jennings, of the Division of Graduate Education at NSF, for keeping us informed of the developments in the IGERT program. We thank Peter Dorhout, Jim Martin, Brian Tissue, Stan Whittingham, Gary Wnek and Mike Ward for their input and for useful discussions.

VI. Panel on Facilities and Resources - T. M. Swager, Coordinator; F. Bates, D. Bishop, J. Jorgensen, T. Marks

The useful scientific lifetime for a piece of equipment is at most ten years and the NSF should be replacing at least 10% of the current equipment base every year if the scientific infrastructure is not to become obsolete.

The commentary offered below is based both on deliberations by the Panel that considered various aspects of Facilities and Resources, and on input by attendees at the Workshop, during as well as after, the formal discussions.

New Opportunities. New and untested ideas are critical to the evolution of science. In recognition of this potential NSF has established an important mechanism to support speculative research through the Small Grant for Exploratory Research Program. This program was recently increased from a single year at \$50,000 to \$100,000 in the first year with a potential second year of funding at the level of \$50,000. The expanded nature of this award was received favorably, as it will likely be more effective at initiating changes in the direction of an investigator's program.

Support for Young Professors. NSF has developed very effective mechanisms to support junior faculty. Earlier programs were criticized as "beauty contests" and many individuals felt there is a need for a formal proposal. This has lead to establishment of the NSF CAREER Award, which resembles in many ways a standard NSF grant application, thereby providing the award more credibility. The Workshop participants considered this program to be highly successful.

Grant Size and Mechanisms for the Review of Proposals. Although researchers would welcome increased funding, the Workshop participants expressed a strong consensus that the size of Division of Materials Research grants should not be increased if it would result in fewer grants. NSF has an outstanding record for supporting the best science and maintaining fairness in funding the research proposals they receive. This includes extensive and careful peer review. One effect of the combination of a growing scientific community and nominally constant dollars (considering inflation) in many scientific areas is that the acceptance rate for proposals has decreased. The view is that the success rate for proposals is dangerously low. Any additional pressure on the system would be extremely harmful and would decrease the range of research activities supported, which is presently skillfully balanced by NSF-Division of Materials Research.

The budget restrictions at NSF may have been so severe that the ability to obtain accurate reviews and to select proposals for funding is in danger of being compromised. The panel considered whether the present system of mail reviews was working effectively, in light of the large number of proposals in the system and the low success rate. The problem of a single reviewer who is asked to evaluate a proposal in isolation without available comparative rankings is becoming severe. A reviewer by himself or herself never knows where the threshold is in any given competition and is faced with the decision of either giving the proposal an excellent rating or running the risk of rejecting it with a less than excellent mark. This issue was discussed extensively by both the sub-panel and the Workshop as a whole. Neither the present system of individual mail reviews nor the establishment of panels of experts was strongly endorsed. The community at large seemed to prefer an intermediate approach whereby proposals would be reviewed by individual reviewers in batches. This would permit comparison of related projects. However, concerns were raised as to whether the reviewers should be asked to rank order proposal merit. Such ranking could not take into account variations in quality between groups of proposals handled by different reviewers. It was felt by the Workshop participants that the batch review process would have the benefits of both of the current systems and while minimizing the drawbacks of each.

Predoctoral and Postdoctoral Fellowships.

Fellowships represent an important mechanism for funding innovative new research, and maintaining NSF's commitment to education. Graduate students and postdocs with fellowship support generally have more flexibility in their choice of research projects and/or research groups. However, predoctoral fellowships are extremely competitive, with a success rate of only approximately 15%. The flexibility provided by the fellowships is important to allow these young scientists realize their true scientific potential.

The Division of Materials Research has never established a Postdoctoral program. The Workshop voted overwhelmingly to recommend that the Division establish a Postdoctoral Fellowship program. It is perceived that such a move will be critical for establishing the next generation of academic researchers.

The NSF has established cooperative relationships with the Office of Naval Research and the Environmental Protection Agency for joint support of research. An expansion of these types of activities may offer new opportunities to expand fellowship support. The Department of Education has a program entitled Graduate Assistance in Areas of National Need (GAANN) which has been used to support graduate students at a number of departments in the country. Interest expressed by other agencies for establishment of graduate fellowships represents an opportunity for NSF to expand support for basic research and education. NSF should consider cooperative arrangements with other Federal Agencies, such as the Department of Education or Department of Defense to expand fellowship support for graduate students.

Large vs. Small Centers and Single PI vs. Multiple PI Grants. The panel found that the general balance between centers and individual PI grants was appropriate and that the DMR staff was both very well informed and attentive to the needs of the community. The center programs have all been well-reviewed by the peer community. Centers vary widely in size and scope, as is appropriate for the intended research and the needs of each particular scientific constituency. Shared facilities, supported either within NSF-supported centers or in facilities of other agencies (Department of Energy, National Institute of Standards and Technology, etc.) play an invaluable role in leveraging resources and in providing the research community with the most "bang for the buck." The panel did find, however, that information on the capabilities, entry procedures, and user charges for these shared facilities was not always readily accessible. It is recommended that facility

managers be more responsive to these needs. An additional benefit from improved access is the potential for greater industrial use of the facilities, which can provide an important revenue source for support of shared facilities. The panel also recognizes that NSF shared facilities cannot and should not compete with privately owned characterization facilities. The panel found that the menu of instrumentation grant programs available to investigators was varied and intelligently tailored to a variety of needs. The Division of Materials Research is to be congratulated in successfully competing for new Major Research Instrumentation funds for the Division.

Evaluating Cost vs. Benefit. Defining the appropriate metrics for evaluating scientific quality (science citation index, number of publications, patents, number of PhD's produced, number of invited lectures, etc.) is an age-old, contentious problem. The panel feels that the Division of Materials Research is very sensitive to this issue, and that a good mix of peer review processes are employed by the Division in the rating/funding decision-making process. The panel feels that no major changes, other than occasional fine-tuning, are necessary.

In regard to the value to society and long-term vs. short-term impact of Division of Materials Research-supported research, the panel has no recommendations for improved evaluation of such contributions, other than previous Division of Materials Research-sponsored reviews of center programs and the consensus of the peer community.

Optimizing the Use of National Facilities by Division of Materials Research-supported Scientists. National facilities, such as neutron and synchrotron light sources are becoming increasingly important as characterization tools for the entire materials chemistry community. The most recent statistics from the US Department of Energy and the National Institute of Standards and Technology research reactor

show that there were 5344 on-site users of the four Department of Energy-operated neutron sources (HFBR, HFIR, IPNS, LANSCE), the four Department of Energy-operated synchrotron sources (SSRL, NSLS, ALS, APS), and the National Institute of Standards and Technology research reactor during FY1997. This number of users is increased a factor of two to three when collaborators who did not actually visit the facilities are included. An analysis of these user populations shows that 46% are associated with Universities compared to 26% from Government laboratories. The dominant scientific disciplines are materials science (37%), life science (26%), and chemical science (12%). Thus, while one cannot specifically separate the materials chemistry community in these user profiles, it is clear that they represent a large fraction of the facility users.

The NSF-Division of Materials Research is already playing a key role in the growth of this large-facility science. They fund two synchrotron sources, SRC and CHESS, several beam lines at other synchrotron sources, and two beam lines at the NIST reactor. These activities are all science based and are supported because of their importance to the mission of the Division of Materials Research. In addition, numerous other materials scientists are supported to perform experiments at these facilities, as confirmed by the user statistics cited above.

This development should continue and offers several opportunities for solid state chemists and materials scientists. Because some of the national neutron and synchrotron sources are presently underutilized, there is opportunity to achieve considerable scientific productivity with incremental funding. Most of the facilities are in the position where base-line operating expenses are funded, so that additional funding can be used directly for the construction and operation of productive instrumentation. This is especially true, for example, for the Advanced Photon Source, where beam lines are currently being constructed.

The next-generation neutron source for the United States, the Spallation Neutron Source, scheduled to be built at Oak Ridge National Laboratory, is on the brink of receiving construction funds. Much of the instrumentation will be funded by the US Department of Energy as part of the construction project. Now is the best time for the solid state and materials chemistry community to influence the instrument design choices and to ensure that their future needs are met.

As another important step, the capabilities of these neutron and synchrotron sources should be made available to the entire solid state and materials chemistry community, moving beyond those who operate beamlines or submit specific research proposals. The creative use of remote access should allow neutron and synchrotron X-ray scattering to become routine characterization tools in the hands of all solid state and materials chemists. This requires paradigms for accessing these facilities other than through peer-reviewed proposals that necessarily create delays in performing experiments. Initial efforts to meet these routine needs of the user community, for example, the "fast-access" modes of performing experiments at IPNS and the National Institute of Standards and Technology reactor, illustrate that the facilities are likely to welcome input about their accessibility and response modes.

Possible New Facility/Equipment Initiatives. A number of new facilities and new pieces of equipment were discussed by both the sub-panel and the Workshop as a whole. Suggestions for new directions included:

- a) increasing support for the development of phase diagrams
- b) computer facilities to increase the level of theoretical analysis in the average paper in this field
- c) new vapor deposition tools to facilitate the fabrication of thin films samples, such as a molecular beam epitaxy facility for chemical synthesis

- d) extreme conditions for both fabrication as well as measurement, such as high pressures, high temperatures, low temperatures, high magnetic fields, etc.
- e) induction furnaces for cold crucible growth techniques
- f) 900 MHz Nuclear Magnetic Resonance system for use at the National Magnet Laboratory,
- g) combinatorial synthesis/screening facilities.

A universally expressed need was for equipment in the \$20,000-100,000 range which falls below what can be asked for in a special equipment proposal and is larger than what can usually be accommodated in a grant which averages less than \$100,000/year. It was suggested that the NSF consider a way to facilitate the acquisition of such pieces of equipment which are becoming mandatory in any modern laboratory. The issue of equipment acquisition and maintenance was generally felt to be a rate-limiting step in scientific progress and was thought to be a problem which should be addressed in a new initiative. As a way of deciding whether this is really a problem for the community as a whole or it is merely the perception of a few members of the panel, the following exercise was recommended: In any functioning, successful business, capital purchases are determined by the need to replace the capital plant on a time scale consistent with its lifetime. For example, with a useful scientific lifetime of ten years at most for a piece of equipment, the NSF should be replacing at least 10% of the current equipment base every year if the scientific infrastructure is not to become obsolete. The panel asks the NSF to determine if its capital equipment purchases are greater or less than this amount, as a way of determining whether a new equipment initiative is warranted.

Other issues discussed by the panel were whether NSF should: a) provide additional staff support for user facilities, b) increase the requirements for university support for grants,

c) and require those with NSF purchased equipment to share it with the community at large. The view of the panel was that there was not a sufficient consensus of the Workshop to warrant any change in present NSF policy.

**VII. Panel on Defining What is Materials Chemistry -
S. I. Stupp, Coordinator; P. Alivisatos, L.
Interrante, J. Moore.**

...materials chemistry has become a new branch of science that will continue to develop into the next century, driven by new or improved technologies that depend on designs involving molecular scales.

This panel was organized to answer the question "What is the intellectual scope of materials chemistry?" and to delineate the relations between materials chemistry and other well established disciplines such as materials science, chemical engineering, and solid state chemistry. The general view was that the subject matter is a discipline concerned with the understanding and control of functional condensed matter from a chemical perspective. Several elements of materials as functional substances were discussed; for example:

- the critical role played by processing in the functionality of materials;
- their variability of composition, which ranges from elemental substances to highly complex mixtures;
- the profound effects that defects and morphology have on their properties.

It was recognized that the nature of materials utilized by society changes with time. Materials chemistry evolves largely by increasing interactions with all the subdisciplines of chemistry, while at the same time some fundamental aspects of

solid state chemistry develop independently of materials chemistry. It was generally agreed that the synthetic aspects of materials cannot be considered in isolation; rather, the interface between materials science and engineering and materials chemistry is an evolving interdisciplinary activity which is experiencing rapid growth. Nonetheless, some of the audience expressed their concern that functionality need not be an essential component in the definition of what constitutes materials. Others felt that materials chemistry and solid state chemistry were one and the same. However, both panelists and audience agreed that materials chemistry is an exciting area of scientific opportunity which will profoundly impact the technological aspects of our society.

Establishment of a definition of materials chemistry is a challenge because of the difficulty in defining what materials are. In the technical arena materials are recognized as matter used to construct the devices and macroscopic structures of a highly developed technology, particularly in areas such as transportation, communication, information, infrastructure, consumer goods, and health care. Nature constructs highly functional devices and complex macroscopic as well; hence a great deal of materials chemistry is to be learned from biology. Since the objective of materials chemistry is to use substances to build devices and macroscopic structures, materials chemistry cannot be developed in isolation from related areas of endeavor. One must also often integrate organic and inorganic matter in a controlled manner in a materials system. Therefore, the materials chemist must be familiar with all branches of chemistry, particularly the less traditional ones, such as polymer chemistry and solid state chemistry. At present, it seems safe to state that materials chemistry has become a new branch of science that will continue to develop into the next century, driven by new or improved technologies that depend on designs involving molecular scales. The new science and technical capabilities will probably develop at the interfaces

between the current technologies and in areas where the knowledge base is expanding rapidly, such as: the interface between information age technology and molecular biology, or between materials processing and frontier synthetic chemistry, or environmental technologies at the interface between materials science and the biological sciences. In all these and others not mentioned here materials chemistry materials chemistry plays a key role because such interdisciplinary activities rely very heavily on the synthesis of chemical structures and on nanotechnology dictated by design needs. We now examine some supporting evidence for the rising importance of materials chemistry as a new branch of chemistry.

Interest at NSF in materials chemistry dates back to the 1980's; a workshop report published in 1986 identified the field as one of "exceptional opportunity in fundamental science". Some of the promising areas that were identified illustrate further the intellectual scope of materials chemistry. These included the design and synthesis of solids, the mechanisms of reactions in the solid state, chemistry at surfaces and interface chemistry under extreme conditions, and novel chemistry relevant to materials processing. The above listings are still valid today. Of particular importance to the definition of the field is the design aspects in the synthesis of solids, as is also emphasized elsewhere in the present Report. This chemical objective cannot be pursued independently of our knowledge base in physics, materials science, engineering, and biology as related to biomolecular structures and biomimetic materials. In response, the NSF has established several special programs over the past decade such as Materials Chemistry, Materials Chemistry and Chemical Processing, and Materials Synthesis and Processing. These funding opportunities reflect the interests of leading academic institutions which are, in turn, excellent sensors of current industrial interests and research and development activities. Industrial research and development is not always involved with long term goals and

is not generally visionary in nature, particularly in the current downsized state of industrial science. Current industrial practice does reflect near future needs and thus, technological pathways that are likely to become prominent in a few years. This is therefore an area in which academia can play a very useful supportive role, particularly regarding longer range objectives.

Another important indicator of the still emerging interest in materials chemistry is to be found in the literature. In 1989 the American Chemical Society initiated the journal *Chemistry of Materials* which is still experiencing a steady growth in the publication of papers. This Journal was actually preceded by a European publication entitled *Materials Chemistry*, currently known as *Materials Chemistry and Physics*. Other journals initiated since then include *Advanced Materials* and *Journal of Materials Chemistry*. The success of these publications reflects the large increase in faculty at universities in the United States and abroad whose main research interests lie in the field of materials chemistry. In some subareas such as polymer science, the number of faculty has increased by a factor of five over the last two decades; most of this increase since 1985 has occurred in chemistry departments. Adequate funding of these research activities should be a high priority in Government agencies supporting research.

The need for growth in materials chemistry research and student training is clearly demonstrated by the current operation of the chemical industry and its projected future activities. A recent report published in *Chemical and Engineering News* contains tabulations of chemical sales for the top 100 companies in the US. The top six companies (DuPont, Dow Chemical, Exxon, General Electric, Union Carbide, and Amoco) all support considerable research efforts reflecting their interest in materials. The number of companies among the top 100 whose products are mainly related to materials chemistry can be conservatively estimated to be as high as one third. In terms

of chemical sales the majority of these companies (60%) rank among the top 50. The report showed, however, that chemical sales have grown only moderately among the top 100 companies since 1995. However, a large majority of companies with a significant activity in materials chemistry experienced an increase in sales, some to an extent well above the average in the industry. An extremely important factor not captured in this report is that at the turn of the 21st century one can expect the continuing emergence of many small high technology companies concerned with materials chemistry based products. On the basis of current trends this growth may well occur in areas involving information age technology and biomedical and environmental technologies. Therefore, the NSF should address the critical funding needs for expansion of research activities and of the educational efforts (as discussed elsewhere in this report) in the field of materials chemistry.

Acknowledgment: The author is grateful to Dr. Norbert Bikales for providing some of the information presented in this article.

ACKNOWLEDGMENTS

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Electronic copies (pdf files) of this report may be found at the following web sites or by the pointers thereon:

<http://www-chem.ucdavis.edu/groups/kauzlarich/dmr/>

<http://www.nsf.gov/mps/dmr/solid.htm>

APPENDIX

Appendix A. Workshop Development and Organization.

Preliminary planning for the Workshop began at the Gordon Research Conference in Solid State Chemistry at New London, NH in July 1996. A Planning Committee for the Workshop was then formed. A subgroup of this Planning Committee convened at the Materials Research Society meeting in Boston on December 5, 1996 to lay the groundwork. The full Committee met on January 25, 1997 in Chicago to draw up concrete plans for the Workshop. The Planning Committee consisted of:

J. K. Burdett, University of Chicago
F. J. DiSalvo, Cornell University
J. M. Honig, Purdue University, chair
S. M. Kauzlarich, University of California, Davis
T. E. Mallouk, Pennsylvania State University, Secretary
D. W. Murphy, Lucent Technology
D. L. Nelson, National Science Foundation, ex officio
S. I. Stupp, University of Illinois, Champaign-Urbana
T. W. Swager, Massachusetts Institute of Technology
M. D. Ward, University of Minnesota

After the untimely death of J. K. Burdett, his place was taken by S. Lee, University of Michigan.

The Workshop was set up with reference to the guiding principles enumerated earlier. In response to a request from the Solid State Chemistry and Materials Planning Committee, D.L. Nelson coordinated the drafting of a set of charges with members of the Division of Materials Research Management Coordinating Team. This set was subsequently coordinated with the Directorate for Mathematical and Physical Sciences before being further considered by the Interagency Liaison Group.

The Workshop agenda were refined and finalized at a subsequent meeting of the Planning Committee (in the absence of J. K. Burdett and F. J. DiSalvo who had other commitments) at the American Chemical Society meeting in San Francisco in April 1997, based on inputs from the Solid State Chemistry and Materials community. Information about the projected Workshop was disseminated at the Gordon Research Conference on Solid State Chemistry at Oxford, England, in September 1997, at which further commentary by the Solid State Chemistry and Materials community, especially from the overseas contingents, was sought. F. J. DiSalvo subsequently generated lists of workers in the Solid State Chemistry and Materials community who were affiliated with academia, industry, and government. These individuals were notified by e-mail about the planned Workshop and invited to comment on the proposed Workshop agenda. The same information was publicized at a web site generated for this purpose by S. M. Kauzlarich. Responses were compiled and distributed to the Planning Committee by J. M. Honig. Thus, considerable effort was devoted to the accumulation of feedback from the community before the Workshop took place. The final program was relayed to the Solid State Chemistry and Materials community via e-mail and the web site. Individual scientists were encouraged to participate in the Workshop proceedings, and those attending the Workshop were asked to register at the Workshop site.

The preparation of the final report was completed after lengthy consultations between J.M. Honig and members of the Planning Committee in February - May 1998. The final report was compiled and prepared by P. K. Dorhout at Colorado State University May - August, 1998. The present document is the product of the above-mentioned operations.

Appendix B. References from the Panel on Education.

1. Explorations of Materials Science, a module developed by General Atomics, San Diego, has been extensively field tested. Parts of this module are included in the booklet based on the ACS Satellite Television (see item 5 below). Additional information is available from Ms. Patricia Winter, Education Outreach Coordinator, General Atomics, P.O. Box 85608, San Diego, CA 92186-9784 (tel. 619-455-3335); winters@vaxd.gat.com

Line of Resistance Kit, ICE (Institute for Chemical Education) - graphite pencil is used to draw electrical circuits to investigate resistivity; an experiment with a piezoelectric crystal is also included

Seeing the Light: The Physics and Materials Science of the Incandescent Light Bulb - this is being developed to be in alignment with the Benchmarks and Standards

2. Interfaces, a brochure provided by the National Science Foundation which provides a general description of educational activities within the Materials Research Science and Engineering Centers.

3. National Science Foundation Science and Technology Centers (STC's) <http://www.nsf.gov/od/osti/centers/stcaward.htm>

Materials Research Science and Engineering Centers (MRSEC's) <http://www.nsf.gov/mps/dmr/mrsec.htm>

4. A complete listing of all the Universities surveyed, along with courses offered is available upon request from S. M. Kauzlarich (smkauzlarich@ucdavis.edu).

5. Products include:

- Text for teachers, "Teaching General Chemistry: A Materials Science Companion" ("Companion") A matrix assists in finding solid-state examples for traditional topics covered in general chemistry. Laboratory experiments, demonstrations, and supplier list.
- "Solid State Resources," CD-ROM, JCE: Software; provides ~100 animations and film clips based on the Companion text.
- Institute for Chemical Education Solid State Model Kit. Permits the facile construction of approximately 80 common structures using rods, templates, and 4 sizes of spheres in radius ratios.
- Institute for Chemical Education Optical Transform Kit. Provides four 35-mm slides, each containing 8 different arrays of dots that permits the user to mimic the essential features of the X-ray diffraction experiment using only a small laser.
- "Teaching Chemistry, 1994. A Materials Science Anthology." American Chemical Society Satellite Television Seminars (videotape and resource booklet with many other leads to instructional materials).

6. <http://www-chem.ucdavis.edu/groups/kauzlarich/dmr/>

APPENDIX C. Program of the Workshop on the Present Status and Future Developments of Solid State Chemistry and Materials.

All meetings were held at NSF Headquarters, 4201 Wilson Boulevard, Arlington, VA 22230

Thursday, January 15, 1998

Room 375

08:30 Welcoming Remarks, T. Weber, National Science Foundation
Workshop Organization, J. M. Honig, Purdue University

Topical Presentations

08:45 **T1.** The Discovery of New Materials Discoveries, R. Cava, Princeton University, Coordinator
R. Haushalter, M. Kanatzidis

09:45 **T2.** Structure-Property Relationships, Steven Lee, University of Michigan, Coordinator
M. Greenblatt, T. Hughbanks, A. Rappe

10:45 COFFEE BREAK

11:15 **T3.** Hybrid Materials, M. D. Ward, University of Minnesota, Coordinator
T. Bein, G. Stucky, M. Tirrell, O. Yaghi

12:15 LUNCH

13:45 Remarks by R. Eisenstein, National Science Foundation

14:00 **T4.** Societal Needs and Technological Opportunities, D. W. Murphy, Lucent Technologies, Bell Laboratories, Coordinator
A. Sleight, T. Vanderah, S. Whittingham

Discussion Groups

15:00 - 17:00

Room 360	Topic 1, Cava
Room 365	Topic 2, Lee
Room 370	Topic 3, Ward
Room 375	Topic 4, Murphy

Panel Preparations Meetings

16:00 - 18:00

Room 380	Panel 1, Kauzlarich (see below)
Room 390	Panel 2, Stupp (see below)
Room 1060	Panel 3, Swager (see below)

Preparations of Report Outlines

20:00 - 21:30

Room 375 Preliminary presentations by coordinators on their findings (Topical presentations) or preparations (panel discussions for Friday, below).
T. E. Mallouk, Pennsylvania State University, Chair

Friday, January 16, 1998

Room 375

Panel Discussions

08:45	P1. Education and Training S. M. Kauzlarich, University of California, Davis, Coordinator J. Chan, A. Ellis, M. Geselbracht, B. Reisner, A. Stacy
09:45	P2. What is Materials Chemistry? S. I. Stupp, University of Illinois, Urbana, Coordinator P. Alivisatos, L. Interrante, J. Moore
10:45	COFFEE BREAK
11:15	P3. Facilities and Resources, T. M. Swager, Massachusetts Institute of Technology, Coordinator F. Bates, D. Bishop, J. Jorgenson, T. Marks

12:15 LUNCH

Preparation of Draft of Report Outlines

14:45 Coordinators, topic presentors, and panelists assemble to prepare a draft report in their own areas.

Same Room Assignments as for Thursday Afternoon

Saturday, January 17, 1998

Room 1060

Preliminary Drafting of Report

08:30 - 12:00 Planning Committee assembles to finalize draft of report, J. M. Honig, Purdue University, Chair, R. Cava, S. M. Kauzlarich, S. Lee, T. E. Mallouk, D. W. Murphy, D. L. Nelson (ex officio), S. I. Stupp, T. M. Swager, M. D. Ward.

APPENDIX D. Listing of Registered Workshop Attendees

Participants in Workshop Presentations:

P. Alivisatos, University of California, Berkeley
F. Bates, University of Minnesota
T. Bein, Purdue University
D. Bishop, Lucent Technologies
R. Cava, Princeton University
J. Chan, University of California, Davis
F. DiSalvo, Cornell University
R. Eisenstein, National Science Foundation
A. Ellis, University of Wisconsin, Madison
M. Geselbracht, Reed College
M. Greenblatt, Rutgers University
R. Haushalter, Symyx
J. Honig, Purdue University
T. Hughbanks, Texas A&M University
L. Interrante, Rensselaer Polytechnic Institute
J. Jorgensen, Argonne national Laboratory
M. Kanatzidis, Michigan State University
S. Kauzlarich, University of California, Davis
S. Lee, University of Michigan
T. Mallouk, Pennsylvania State University
T. Marks, Northwestern University
J. Moore, University of Illinois, Urbana-Champaign
D. Murphy, Lucent Technologies
D. Nelson, National Science Foundation
A. Rappe, University of Pennsylvania
B. Reisner, University of California, Berkeley
A. Sleight, Oregon State University
A. Stacy, University of California, Berkeley
G. Stucky, University of California, Santa Barbara
S. Stupp, University of Illinois, Urbana-Champaign
T. Swager, Massachusetts Institute of Technology
T. Vanderah, National Institute of Standards and Technology
M. Ward, University of Minnesota
T. Weber, National Science Foundation
S. Whittingham, State University of New York, Binghamton
O. Yaghi, Arizona State University

Attendees Who Registered at the Workshop:

R. Bedard, Universal Oil Products
F. Chen, Ryder College
J. Corbett, Iowa State University
P. Dorhout, Colorado State University
L. DuBois, Defense Advanced Research Projects Agency
J. Ibers, Northwestern University
A. Jacobson, University of Houston
W. Jones, State University of New York, Binghamton
P. Kaszynski, Vanderbilt University
S. Keller, University of Missouri, Columbia
R. Kelley, Department of Energy
M. Kertesz, Georgetown University
J. Li, Rutgers University, Camden
J. Martin, North Carolina State University
L. Montgomery, Indiana University
C. Murray, International Business Machines, Watson
D. Neumann, National Institute of Standards and Technology
J. Pazik, Office of Naval Research
K. Poeppelmeier, Northwestern University
R. Reeber, Army Research Office
S. Sun, International Business Machines, Watson
B. Tissue, Virginia Polytechnic Institute
B. Toby, National Institute of Standards and Technology
Z. Zhang, Georgia Institute of Technology

**APPENDIX E. Listing of Individuals Who Provided
Written Commentary Concerning the Workshop Organization.**

The individuals listed below provided written commentary to assist the Planning Committee in delineating the Workshop objectives. Due to a computer malfunction, the listing may not be complete; any omissions are entirely inadvertent.

R. Bedard, Universal Oil Products
T. Beebe, Jr., University of Utah
T. Bein, Purdue University
S. Byrn, Purdue University
M. Cameron, National Science Foundation
J. Corbett, Iowa State University
P. Dorhout, Colorado State University
K. Doxsee, National Science Foundation
F. Fisher, National Science Foundation
G. Girolami, University of Illinois, Urbana-Champaign
J. Goodenough, University of Texas, Austin
C. Grey, State University of New York, Stony Brook
J. Harrington, National Science Foundation
L. Haworth, National Science Foundation
L. Hess, National Science Foundation
S. Hixon, National Science Foundation
J. Ibers, Northwestern University
G. Irene, University of North Carolina
M. Kanatzidis, Michigan State University
R. Kelley, Department of Energy
P. Kumar, National Science Foundation
S. Lapporte, National Science Foundation
A. Lovinger, National Science Foundation
B. MacDonald, National Science Foundation
T. Mallouk, Pennsylvania State University
J. Martin, North Carolina State University
J. McDevitt, University of Texas, Austin
J. Miller, University of Utah
R. Miranda, National Science Foundation
D. Murphy, Lucent Technologies
J. Parise, State University of New York, Stony Brook
J. Pazik, Office of Naval Research
W. Pickett, University of California, Davis
H. Richtol, National Science Foundation
J. Toulouse, National Science Foundation
J. Tour, University of South Carolina
T. Vanderah, National Institute of Standards and Technology
M. Ward, University of Minnesota
R. Wellek, National Science Foundation
S. Whittingham, State University of New York, Binghamton.